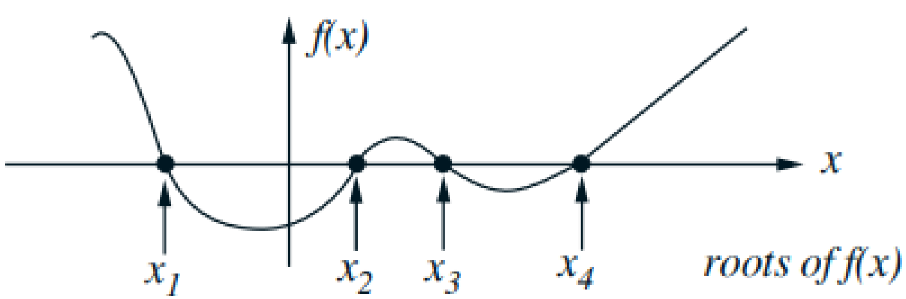
Roots of non-linear Equation

SOLVING FOR ROOTS OF NONLINEAR EQUATIONS

- Consider the equation

$$f(x) = 0$$

- Roots of equation f(x) are the values of x which satisfy the above expression. Also referred to as the zeros of an equation



Methods to find Roots of quadric equation

1. Direct Method

$$f(x) = ax^2 + bx + c = 0$$

To solve

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

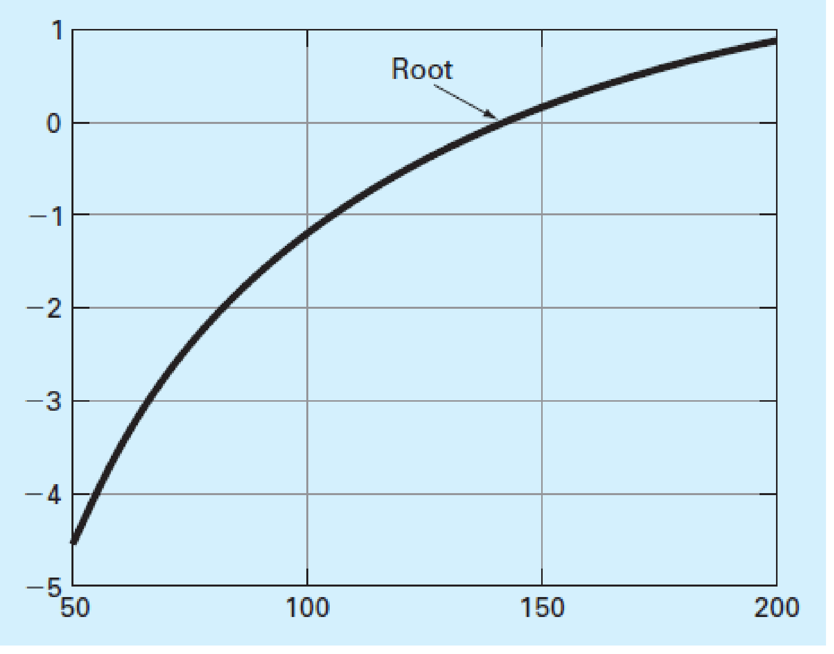
There are many other functions for which the root cannot be determined so easily. Before the advent of digital computers, there were a number of ways to solve for the roots of such equations. For some cases, the roots could be obtained by direct methods as shown in above equation. There are many more that could not. In such instances, the only alternative is an approximate solution technique.

Approximation

1. One method to obtain an approximate solution is to plot the function and determine where it crosses the *x axis.* Although graphical methods are useful for obtaining rough estimates of roots, they are limited because of their lack of precision.
2. An alternative approach is to use *trial and error.* This technique consists of guessing a value of *x and evaluating whether f (x) is* zero.
3. Numerical methods represent alternatives that are also approximate but employ systematic strategies.

GRAPHICAL METHODS

- A simple method for obtaining an estimate of the root of the equation *f (x) = 0 is to make* a plot of the function and observe where it crosses the *x axis. This point, which represents* the *x value for which f (x) = 0, provides a rough approximation of the root.*



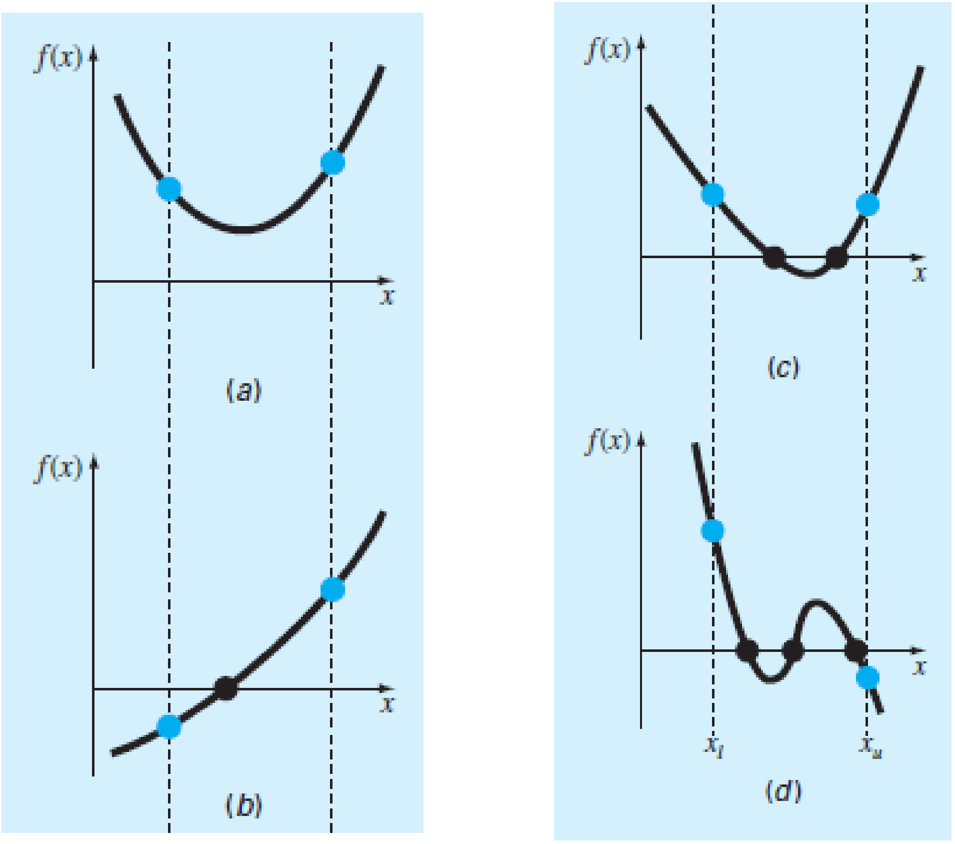
- The two major classes of methods available are distinguished by the type of initial guess.

1. *Bracketing methods. As the name implies, these are based on two initial guesses that* bracket the root , that is, are on either side of the root.
2. *Open methods. These methods can involve one or more initial guesses, but there is no* need for them to bracket the root.

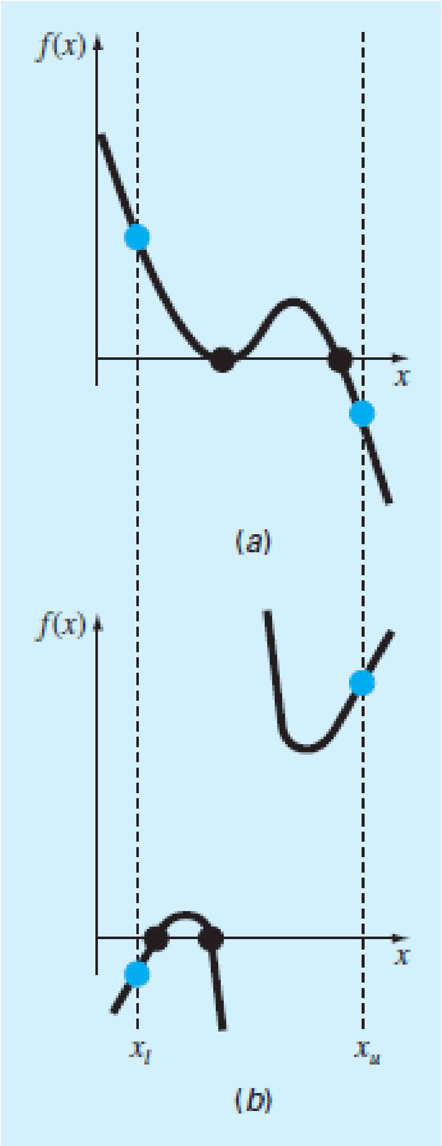
note

- For well-posed problems, the bracketing methods always work but converge slowly
- In contrast, the open methods do not always work (i.e., they can diverge), but when they do they usually converge quicker.

Number of general ways that a root may occur in an interval prescribed by a lower bound *xl and* an upper bound *xu*



exceptions to the general cases depicted



Incremental Search Method

incsearch(m function)*:- For the problems which are* compounded by the possible existence of multiple roots

- *Incremental search methods capitalize on this observation by locating an interval* where the function changes sign.
- A potential problem with an incremental search is the choice of the increment length.
- If the length is too small, the search can be very time consuming.
- On the other hand, if the length is too great, there is a possibility that closely spaced roots might be missed

Tutorial example 1

Find out the roots for identified brackets within the interval [3, 6] for the function:

$$f\,(x) = \sin(10x) + \cos(3x)$$

Bisection method

- It is the first numerical method developed to find the root of a nonlinear equation f(x)=0 was the bisection method, also called binary-search method.

Theorem:

❑ An equation *f(x)=0,* where *f(x)* is a real continuous function, has at least one root between x_l and x_u if (See Figure 1).

$$f(x_l)\,f(x_u) < 0$$

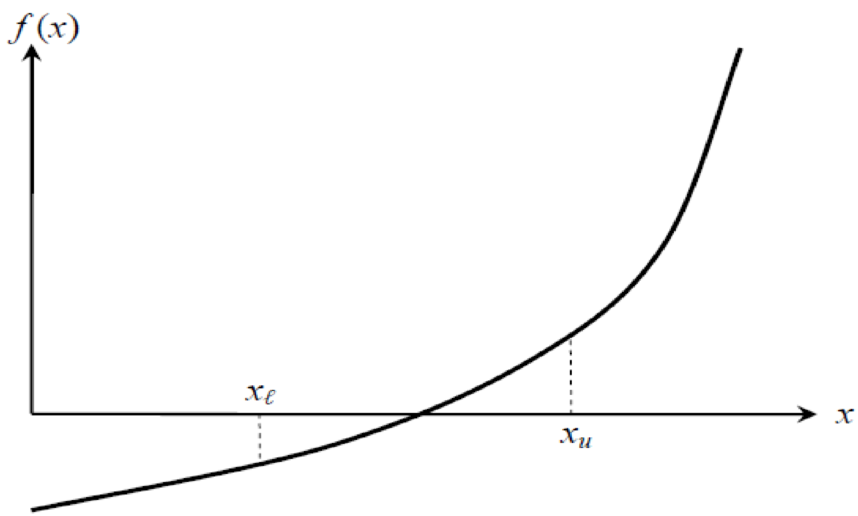


Figure 1: At least one root exists between the two points if the function is real, continuous, and changes sign.

Continue.....

- Note that if $f(x_l)\,f(x_u) > 0$, there may or may not be any root between x_l and x_u (figure 2 and 3)

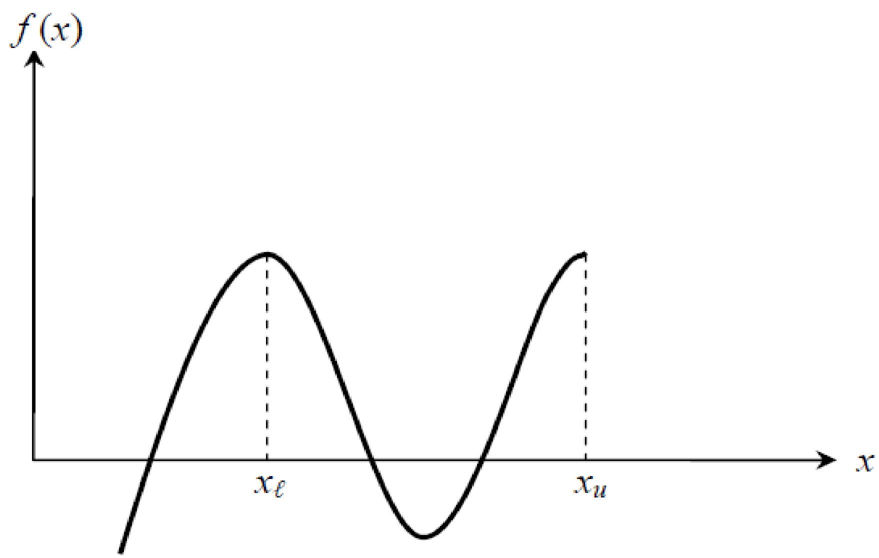


Figure 2: If the function *f(x)* does not change sign between the two points, roots of the equation *f(x)=0* may still exist between the two points.

Continue.....

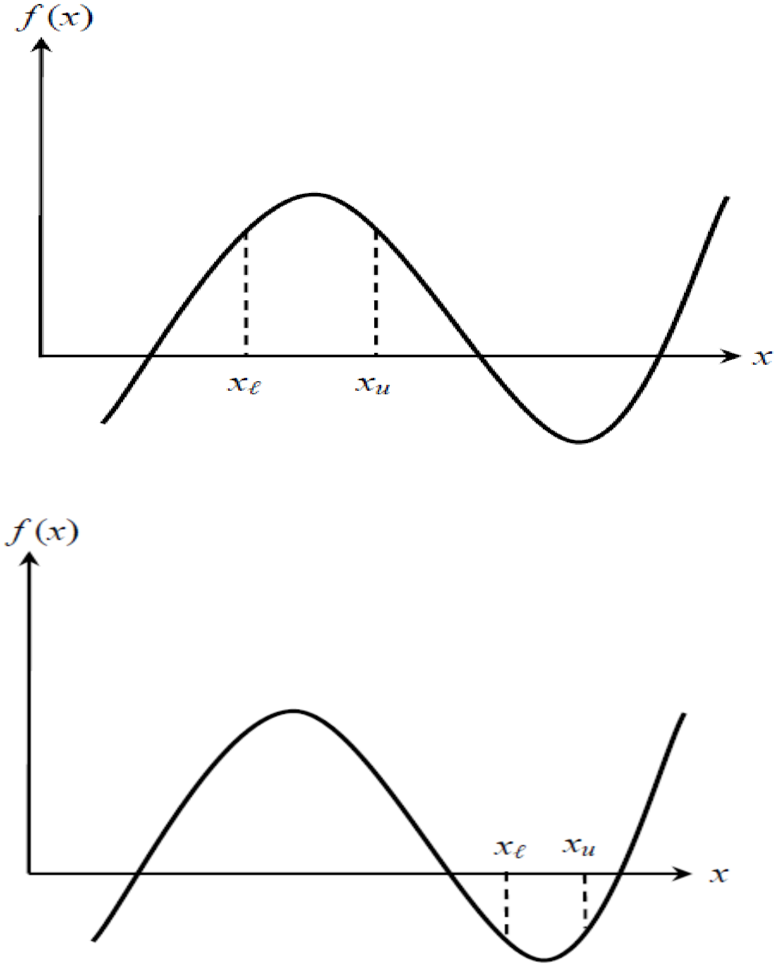


Figure 3: If the function *f(x)* does not change sign between the two points, there may not be any roots of the equation *f(x)=0* exist between the two points.

Continue.....

- If $f(x_l)f(x_u) < 0$, then there may be more than one root between x_l and x_u
Figure 4).

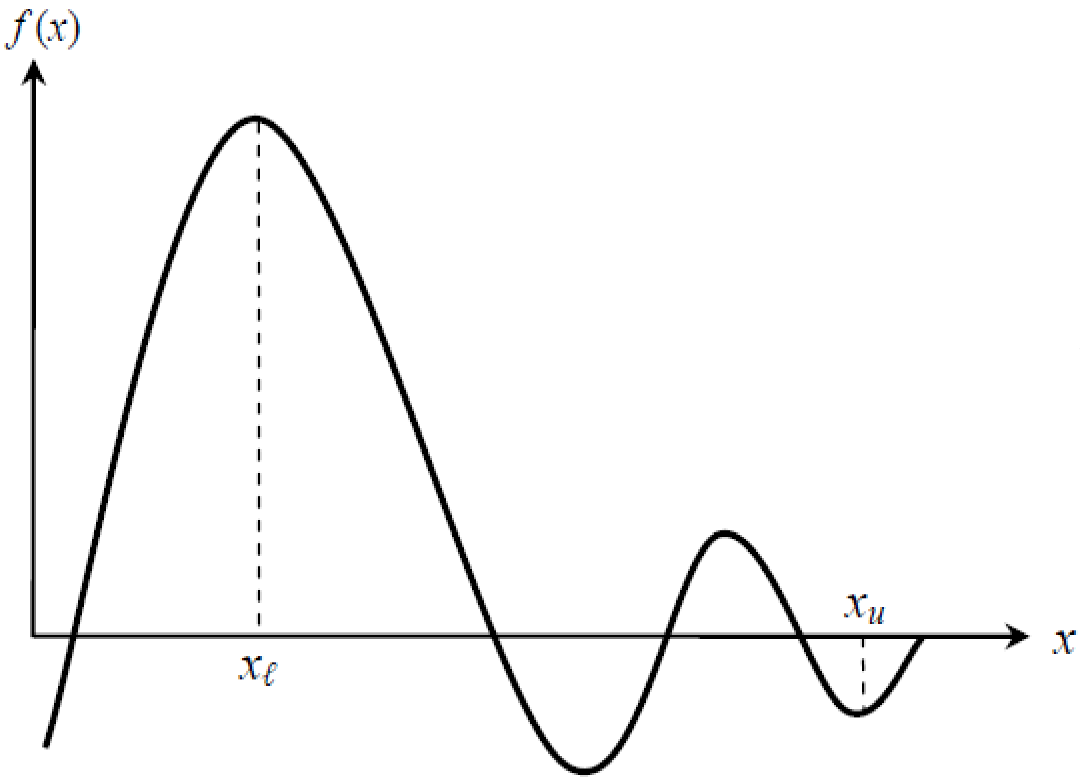


Figure 4: If the function *f(x)* changes sign between the two points, more than one root for the equation *f(x)=0* may exist between the two points.

Continue.....

Theorem only guarantees one root between the root between x_l and x_u.

Since the root is bracketed between x_l and x_u, we find the midpoint, x_m, of x_l and x_u. This gives us two new intervals,

1. x_l and x_m and
2. x_m and x_u

- Is the root now between x_l and x_m or between x_m and x_u?

Answer : Find the sign of $f(x_l)f(x_u) < 0$, then the root is between x_l and x_m otherwise, it is between x_m and x_u.

As we repeat this process, the width of the interval x_l and x_m becomes smaller and smaller.

Continue.....

Algorithm:

The algorithm for bisection method is given as follows:

1) Choose x_l *and* x_u, as two guesses for the root such that $f(x_l)f(x_u) < 0$ or in other words, *f(x)* changes sign between x_l *and* x_u.

2) Estimate the root , x_m , of the equation *f(x)=0* the mid-point between x_l and x_u as,

$$x_m = \frac{x_l + x_u}{2}$$

3) Now check the following:

a) If $f(x_l)f(x_u) < 0$, then the root lies between x_l and x_m ;
then $x_l = x_l$ and $x_m = x_u$.

b) If $f(x_l)f(x_u) > 0$, then the root lies between x_m and x_u ;
then $x_m = x_l$ and $x_u = x_u$.

c) If $f(x_l)f(x_u) = 0$, then the root is x_m . Stop the algorithm.

Continue…..

4) Find the new estimate of the root,

$$x_m = \frac{x_l + x_u}{2}$$

Find the absolute relative approximate error as,

$$\left|E_a\right| = \left|\frac{x_m^{new} - x_m^{old}}{x_m^{new}}\right| \times 100$$

Where,

x_m^{new} = Estimated root from present iteration

x_m^{old} = Estimated root from previous iteration

5) Compare the absolute relative approximate error $|E_a|$ with the pre-specified relative error tolerance E_s if $|E_a| > E_s$, then go to Step 3, else stop the algorithm.

6) The number of iterations may also be the stopping criteria for termination of the algorithm.

Error

- Human error
- Truncation and Round-off error

- Error estimation
  - Absolute error
  - Relative error
  - Percentage error

Tutorial

1) Find a root of the equation using bisection method correct to three decimal places,

$$f(x) = x^3 - 4x - 9$$

2) Perform five iteration of the bisection method to obtain the smallest positive root of the equation,

$$f(x) = x^3 - 5x + 1$$

3) Find a root of the equation using bisection method correct to three decimal places,

$$f(x) = 3x + \sin x - e^x = 0$$

Tutorial

4) Perform five iteration of the bisection method to obtain the smallest positive root of the equation,

$$f(x) = \cos x - xe^{x} = 0$$

5) Find a root of the equation using bisection method correct to three decimal places,

$$f(x) = x^{3} - x - 4 = 0$$

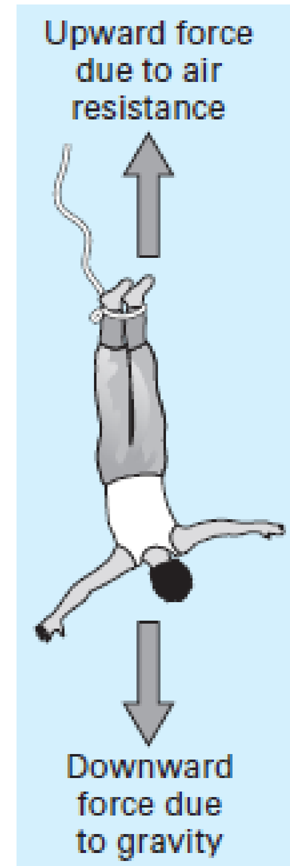
Assignment 1

- Use the graphical approach to determine the mass of the bungee jumper with a drag coefficient of 0.25 kg/m to have a velocity of 36 m/s after 4 s of free fall. Note: The acceleration of gravity is 9.81 m/s2.

CASE STUDY: BUNGEE JUMPER VELOCITY

Rate of change of velocity with respect to time

$$\frac{dv}{dt} = g - \frac{c_d}{m}v^2$$



where *v = downward vertical velocity (m/s),*

t = time (s),

g = the acceleration due to gravity (~= 9*.81 m/s2),*

cd = a lumped drag coefficient (kg/m), and

m = the jumper's mass (kg).

Newton-Raphson Method

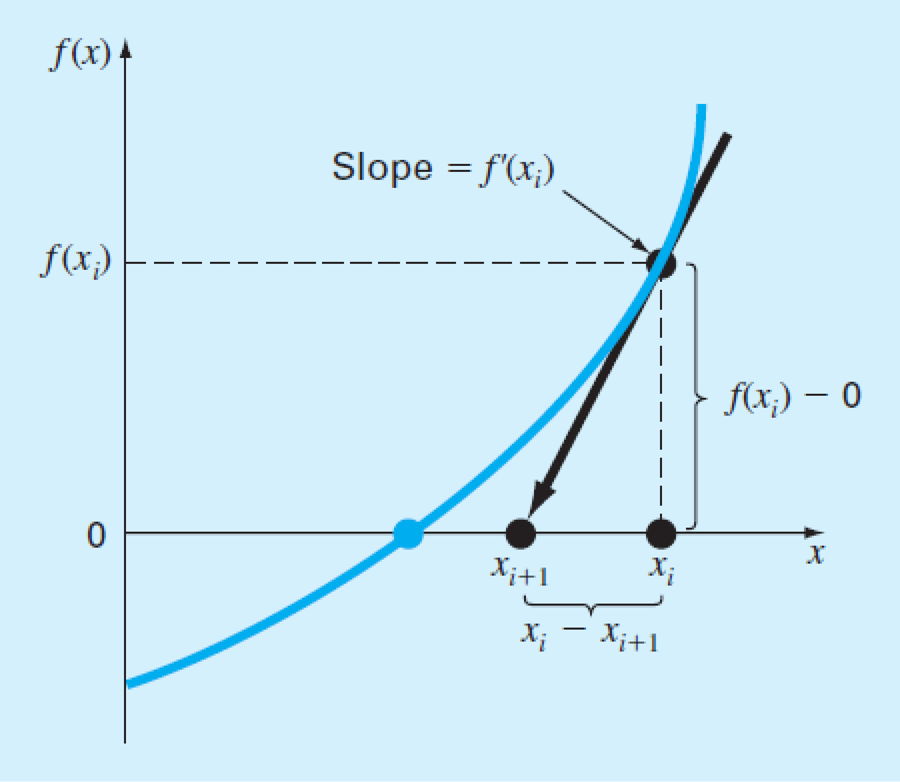
SIMPLE FIXED-POINT ITERATION

- open methods employ a formula to predict the root
- rearrange the function *f (x) = 0 so that x is on the left-hand* side of the equation
- *x = g(x)*
- This transformation can be accomplished either by algebraic manipulation or by simply adding *x to both sides of the original equation.*
- The utility of above Eq. is that it provides a formula to predict a new value of *x as a* function of an old value of *x.*
- Thus, given an initial guess at the root *xi , Eq. can be* used to compute a new estimate *xi+1 as expressed by the iterative formula*
- *xi+1 = g(xi)*
- the approximate error for this equation can be determined using the error estimator

$$\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| 100\%$$

NEWTON-RAPHSON

- If the initial guess at the root is *xi , a tangent can be extended from the point [xi , f (xi)]. The point where this tangent crosses the x axis usually represents an improved* estimate of the root.



Newton-Raphson (Algorithm)

- Start from an initial value x0
- Define iteration

Do $k = 0$ to ….?

$$x^{k+1} = x^k - \left[\frac{df}{dx}(x^k)\right]^{-1} f(x^k)$$ **OR** $$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f^{/}(x_n)}}$$

until convergence

Newton-Raphson Method Advantages

- Convergence is quadratic

- Extremely powerful technique gives solution in minimum iterations

Newton-Raphson Method Disadvantages

- It requires to calculate derivative or Jacobian in case of multiple functions
- Method fails for very small value of derivative as it returns infinite number
- If stationary point, the derivative will be zero and method will terminate due to divided by zero error
- When there are two or more roots that are close together then it may take many iterations before the iterates get close enough to one of them for the quadratic convergence to be apparent

Newton-Raphson Method

1. Find the roots of the equation $f(x) = 5\sin^2 x - 8\cos^5 x = 0$

   Consider $x_0 = 0.5 \; and \; 1.5, \; \varepsilon = 1e-6$

2. Find the roots of the equation $f(x) = e^x - 3x^2 = 0$

   Consider $x_0 = 0.7 \; and \; \varepsilon = 1e-5$

3. Find the roots of the equation $f(x) = x - 2 + \ln(x) = 0$

   Consider $x_0 = 1.5, \; and \; \varepsilon = 1e-5$

4. Find the roots of the equation $f(x) = x^3 - x + 3 = 0$

   Consider $x_0 = -2.0, \; and \; \varepsilon = 1e-5$

Interpolation

Interpolation

- **Interpolation is used to Find Intermediate Data Points From Given Data Set.**

x	F(x)
0	6
1	5
2	6
3	9
4	14
5	21
6	30

Find f(2.5) ?

Linear interpolation, f(2.5)=7.5
Actual, f(2.5)=7.25

The Interpolation Problem

Given a set of n+1 points,

$$\left(x_0, f(x_0)\right), \left(x_1, f(x_1)\right), \ldots., \left(x_n, f(x_n)\right)$$

Find an n^{th} order polynomial $f_n(x)$

that passes through all points, such that:

$$\boxed{f_n(x_i) = f(x_i) \quad for \ i = 0,1,2,\ldots,n}$$

Example

An experiment is used to determine the viscosity of water as a function of temperature. The following table is generated:

Problem: Estimate the viscosity when the temperature is 8 degrees.

Temperature (degree)	Viscosity
0	1.792
5	1.519
10	1.308
15	1.140

Interpolation Problem

Find a polynomial that fits the data points exactly.

$$V(T) = \sum_{k=0}^{n} a_k T^k$$

$$V_i = V(T_i)$$

V : Viscosity

T : Temperature

a_k : Polynomial coefficients

Linear Interpolation: V(T)= 1.73 − 0.0422 T

V(8)= 1.3924

Existence and Uniqueness

Given a set of n+1 points:

$$\left(x_0, f(x_0)\right), \left(x_1, f(x_1)\right), \ldots., \left(x_n, f(x_n)\right)$$

Assumption: $x_0, x_1, \ldots, x_n$ are distinct

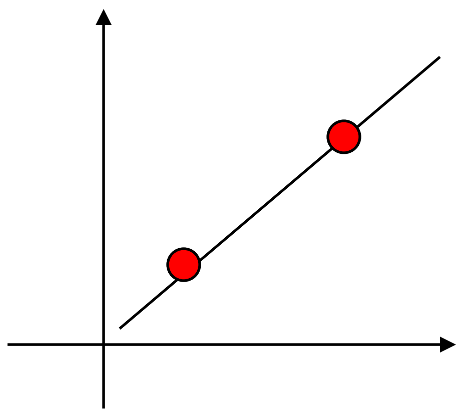
Theorem:

There is a unique polynomial $\boldsymbol{f_n(x)}$ of order $\leq$ n such that:

$$f_n(x_i) = f(x_i) \qquad for \quad i = 0, 1, \ldots, n$$

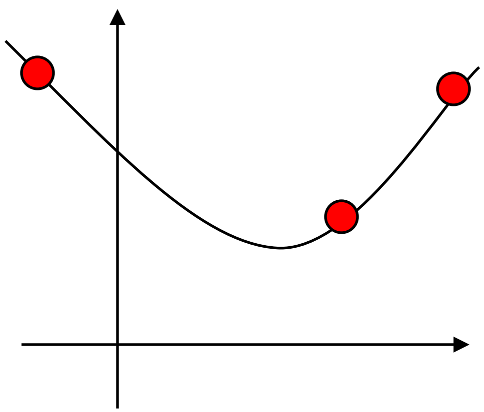
Examples of Polynomial Interpolation

Linear Interpolation



- Given any two points, there is one polynomial of order ≤ 1 that passes through the two points.

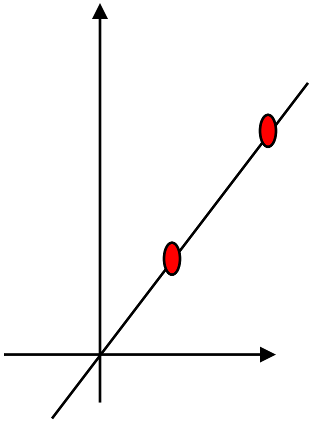
Quadratic Interpolation



Given any three points there is one polynomial of order ≤ 2 that passes through the three points.

Linear Interpolation

Given any two points, $\left(x_0, f(x_0)\right), \left(x_1, f(x_1)\right)$



The line that interpolates the two points is:

$$f_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}\left(x - x_0\right)$$

Example :

Find a polynomial that interpolates (1,2) and (2,4).

$$f_1(x) = 2 + \frac{4-2}{2-1}\left(x - 1\right) = 2x$$

Quadratic Interpolation

- Given any three points: $\left(x_0, f(x_0)\right), \left(x_1, f(x_1)\right), and \left(x_2, f(x_2)\right)$
- The polynomial that interpolates the three points is:

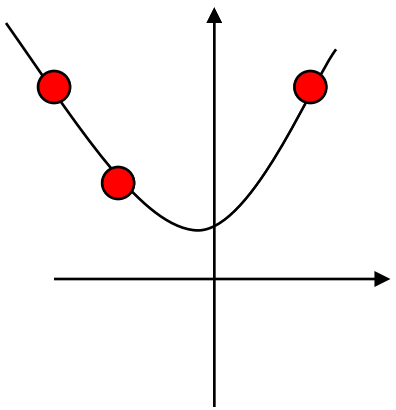
$$\boxed{f_2(x) = b_0 + b_1\left(x - x_0\right) + b_2\left(x - x_0\right)\left(x - x_1\right)}$$

$where:$

$$b_0 = f(x_0)$$

$$b_1 = f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$b_2 = f[x_0, x_1, x_2] = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$



General nth Order Interpolation

Given any n+1 points: $\left(x_0, f(x_0)\right), \left(x_1, f(x_1)\right), \ldots, \left(x_n, f(x_n)\right)$

The polynomial that interpolates all points is:

$$f_n(x) = b_0 + b_1\left(x - x_0\right) + b_2\left(x - x_0\right)\left(x - x_1\right) + \ldots + b_n\left(x - x_0\right)\ldots\left(x - x_{n-1}\right)$$

$$b_0 = f(x_0)$$

$$b_1 = f[x_0, x_1]$$

....

$$b_n = f[x_0, x_1, \ldots, x_n]$$

Divided Differences

$$f[x_k] = f(x_k)$$ Zeroth order DD

$$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0}$$ First order DD

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$$ Second order DD

....

$$f[x_0, x_1, \ldots, x_k] = \frac{f[x_1, x_2, \ldots, x_k] - f[x_0, x_1, \ldots, x_{k-1}]}{x_k - x_0}$$

Divided Difference Table

x	F[ ]	F[,]	F[, ,]	F[, , ,]
x_0	F[x0]	$F[x_0,x_1]$	$F[x_0,x_1,x_2]$	$F[x_0,x_1,x_2,x_3]$
x_1	$F[x_1]$	$F[x_1,x_2]$	$F[x_1,x_2,x_3]$	
x_2	$F[x_2]$	$F[x_2,x_3]$		
x_3	$F[x_3]$			

$$f_n(x) = \sum_{i=0}^{n} \left\{ F[x_0, x_1, \ldots, x_i] \prod_{j=0}^{i-1} \left(x - x_j \right) \right\}$$

Divided Difference Table

x	F[ ]	F[,]	F[, ,]
0	-5	2	-4
1	-3	6	
-1	-15		

x_i	$f(x_i)$
0	-5
1	-3
-1	-15

Entries of the divided difference table are obtained from the data table using simple operations.

Divided Difference Table

x	F[ ]	F[,]	F[, ,]
0	-5	2	-4
1	-3	6	
-1	-15		

x_i	$f(x_i)$
0	-5
1	-3
-1	-15

The first two column of the

table are the data columns.

Third column: First order differences.

Fourth column: Second order differences.

Divided Difference Table

x	F[ ]	F[,]	F[, ,]
0	-5	2	-4
1	-3	6	
-1	-15		

$$\frac{-3-(-5)}{1-0}=2$$

$$f[x_0,x_1]=\frac{f[x_1]-f[x_0]}{x_1-x_0}$$

x_i	y_i
0	-5
1	-3
-1	-15

Divided Difference Table

x	F[ ]	F[,]	F[, ,]
0	-5	2	-4
1	-3	6	
-1	-15		

$$\frac{-15-(-3)}{-1-1}=6$$

$$f[x_1,x_2]=\frac{f[x_2]-f[x_1]}{x_2-x_1}$$

x_i	y_i
0	-5
1	-3
-1	-15

Divided Difference Table

x	F[ ]	F[,]	F[, ,]
0	-5	2	-4
1	-3	6	
-1	-15		

$$\frac{6-(2)}{-1-(0)} = -4$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$$

x_i	y_i
0	-5
1	-3
-1	-15

Divided Difference Table

x	F[ ]	F[,]	F[, ,]
0	-5	2	-4
1	-3	6	
-1	-15		

x_i	y_i
0	-5
1	-3
-1	-15

$$f_2(x) = -5 + 2(x-0) - 4(x-0)(x-1)$$

$f_2(x)$= $F[x_0]+F[x_0,x_1]\,(x-x_0)+F[x_0,x_1,x_2]\,(x-x_0)(x-x_1)$

Two Examples

Obtain the interpolating polynomials for the two examples:

x	y
1	0
2	3
3	8

x	y
2	3
1	0
3	8

What do you observe?

Two Examples

x	Y		
1	0	3	1
2	3	5	
3	8		

$$P_2(x) = 0 + 3(x-1) + 1(x-1)(x-2)$$
$$= x^2 - 1$$

x	Y		
2	3	3	1
1	0	4	
3	8		

$$P_2(x) = 3 + 3(x-2) + 1(x-2)(x-1)$$
$$= x^2 - 1$$

Ordering the points should not affect the interpolating polynomial.

Properties of Divided Difference

Ordering the points should not affect the divided difference:

$$f[x_0, x_1, x_2] = f[x_1, x_2, x_0] = f[x_2, x_1, x_0]$$

Example

- Find a polynomial to interpolate the data.

x	f(x)
2	3
4	5
5	1
6	6
7	9

Example

x	f(x)	f[,]	f[, ,]	f[, , ,]	f[, , , ,]
2	3	1	-1.6667	1.5417	-0.6750
4	5	-4	4.5	-1.8333	
5	1	5	-1		
6	6	3			
7	9				

$$f_4 = 3 + 1(x-2) - 1.6667(x-2)(x-4) + 1.5417(x-2)(x-4)(x-5)$$
$$- 0.6750(x-2)(x-4)(x-5)(x-6)$$

Summary

Interpolating Condition : $f(x_i) = f_n(x_i) \quad for \quad i = 0, 1, 2, ..., n$

* The interpolating Polynomial is unique.

* Different methods can be used to obtain it

  - Newton Divided Difference

  - Lagrange Interpolation

  - Other methods

Ordering the points should not affect the interpolating polynomial.

Examples-Linear

1. Estimate the natural logarithmic of 2 using linear interpolation. First, perform the computation by interpolating between *l_n 1 =0* and *l_n 6= 1.7917*. Then repeat the procedure, but use a smaller interval from l_n 1 to l_n 4. Note that the true value of l_n 2 is 0.6931472.

2. Given *f(2) = 4, f(2.5)=5.5*, Find the linear interpolating polynomial. Find an approximation value of f(2.2)

3. Let *f(x)=in(1+x)*, $x_0=1$ and $x_1=1.1$. Use linear interpolation to calculate an approximate value for *f(1.04)*.

4. For the data points (0.82, 2.270500) and (0.83, 2.293319), find $P_1(x)$ and evaluate $P_1(0.826)$.

5. Obtain an estimate of $e^{0.826}$ using the function values $e^{0.82}$= 2.270500, $e^{0.83}$= 2.293319

Examples-Quadratic

In the following problems, the values of a function f(x) are given . Find the interpolating polynomial that fits the data. Find the approximation to f(x) at the indicated points using this polynomial,

1.

X	*-2*	*-1*	*0*	*1*	*3*	*4*
f(x)	*9*	*16*	*17*	*18*	*44*	*81*

Interpolate at x=0.5 and x=3.1

2.

X	*1*	*3*	*4*	*5*	*7*	*10*
f(x)	*3*	*31*	*69*	*131*	*351*	*1011*

Interpolate at x=3.5 and x=8.0

3.

X	*0*	*1*	*2*	*4*	*5*	*6*
f(x)	*1*	*14*	*15*	*5*	*6*	*19*

Interpolate at x=3.0 and x=5.5

4. .

X	*-1*	*1*	*4*	*7*
f(x)	*-2*	*0*	*63*	*342*

Interpolate at x=5.0

Lagrange Interpolation

The Interpolation Problem

Given a set of n+1 points:

$$\left(x_0, f(x_0)\right), \left(x_1, f(x_1)\right), \ldots., \left(x_n, f(x_n)\right)$$

Find an n^{th} order polynomial: $f_n(x)$

that passes through all points, such that:

$$\boxed{f_n(x_i) = f(x_i) \quad for \ i = 0, 1, 2, \ldots, n}$$

Lagrange Interpolation

Problem:

Given

x_i	x_0	x_1	....	x_n
y_i	y_0	y_1	....	y_n

Find the polynomial of least order $f_n(x)$ such that:

$$f_n(x_i) = f(x_i) \qquad for \quad i = 0,1,\ldots,n$$

Lagrange Interpolation Formula:

$$f_n(x) = \sum_{i=0}^{n} f\left(x_i\right) \ \ell_i(x)$$

$$\ell_i(x) = \prod_{j=0,\, j\neq i}^{n} \frac{\left(x - x_j\right)}{\left(x_i - x_j\right)}$$

Lagrange Interpolation

$\ell_i(x)$ are called the cardinals.

The cardinals are n^{th} order polynomials:

$$\ell_i(x_j) = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

Lagrange Interpolation Example

x	1/3	1/4	1
y	2	-1	7

$$P_2(x) = f(x_0)\ell_0(x) + f(x_1)\ell_1(x) + f(x_2)\ell_2(x)$$

$$\ell_0(x) = \frac{(x-x_1)}{(x_0-x_1)}\frac{(x-x_2)}{(x_0-x_2)} = \frac{(x-1/4)}{(1/3-1/4)}\frac{(x-1)}{(1/3-1)}$$

$$\ell_1(x) = \frac{(x-x_0)}{(x_1-x_0)}\frac{(x-x_2)}{(x_1-x_2)} = \frac{(x-1/3)}{(1/4-1/3)}\frac{(x-1)}{(1/4-1)}$$

$$\ell_2(x) = \frac{(x-x_0)}{(x_2-x_0)}\frac{(x-x_1)}{(x_2-x_1)} = \frac{(x-1/3)}{(1-1/3)}\frac{(x-1/4)}{(1-1/4)}$$

$$P_2(x) = 2\{-18(x-1/4)(x-1)\} - 1\{16(x-1/3)(x-1)\}$$
$$+7\{2(x-1/3)(x-1/4)\}$$

Example

Find a polynomial to interpolate:

Both Newton's interpolation method and Lagrange interpolation method must give the same answer.

x	y
0	1
1	3
2	2
3	5
4	4

Newton's Interpolation Method

0	1	2	-3/2	7/6	-5/8
1	3	-1	2	-4/3	
2	2	3	-2		
3	5	-1			
4	4				

Interpolating Polynomial

$$f_4(x) = 1 + 2(x) - \frac{3}{2}x(x-1) + \frac{7}{6}x(x-1)(x-2)$$
$$- \frac{5}{8}x(x-1)(x-2)(x-3)$$

$$f_4(x) = 1 + \frac{115}{12}x - \frac{95}{8}x^2 + \frac{59}{12}x^3 - \frac{5}{8}x^4$$

Interpolating Polynomial Using Lagrange Interpolation Method

$$f_4(x) = \sum_{i=0}^{4} f(x_i)\ \ell_i = \ell_0 + 3\ell_1 + 2\ell_2 + 5\ell_3 + 4\ell_4$$

$$\ell_0 = \frac{(x-1)}{(0-1)}\ \frac{(x-2)}{(0-2)}\ \frac{(x-3)}{(0-3)}\ \frac{(x-4)}{(0-4)} = \frac{(x-1)(x-2)(x-3)(x-4)}{24}$$

$$\ell_1 = \frac{(x-0)}{(1-0)}\ \frac{(x-2)}{(1-2)}\ \frac{(x-3)}{(1-3)}\ \frac{(x-4)}{(1-4)} = \frac{x(x-2)(x-3)(x-4)}{-6}$$

$$\ell_2 = \frac{(x-0)}{(2-0)}\ \frac{(x-1)}{(2-1)}\ \frac{(x-3)}{(2-3)}\ \frac{(x-4)}{(2-4)} = \frac{x(x-1)(x-3)(x-4)}{4}$$

$$\ell_3 = \frac{(x-0)}{(3-0)}\ \frac{(x-1)}{(3-1)}\ \frac{(x-2)}{(3-2)}\ \frac{(x-4)}{(3-4)} = \frac{x(x-1)(x-2)(x-4)}{-6}$$

$$\ell_4 = \frac{(x-0)}{(4-0)}\ \frac{(x-1)}{(4-1)}\ \frac{(x-2)}{(4-2)}\ \frac{(x-3)}{(4-3)} = \frac{x(x-1)(x-2)(x-3)}{24}$$

Inverse Interpolation
Error in Polynomial Interpolation

Inverse Interpolation

Problem : Given a table of values

Find x such that : $f(x) = y_k$, where y_k is given

x_i	x_0	x_1	....	x_n
y_i	y_0	y_1	....	y_n

<u>One approach</u>:

Use polynomial interpolation to obtain $f_n(x)$ to interpolate the data then use Newton's method to find a solution to x

$$f_n(x) = y_k$$

Inverse Interpolation

<u>**Inverse interpolation:**</u>

1. Exchange the roles of x and y.

x_i	x_0	x_1	....	x_n
y_i	y_0	y_1	....	y_n

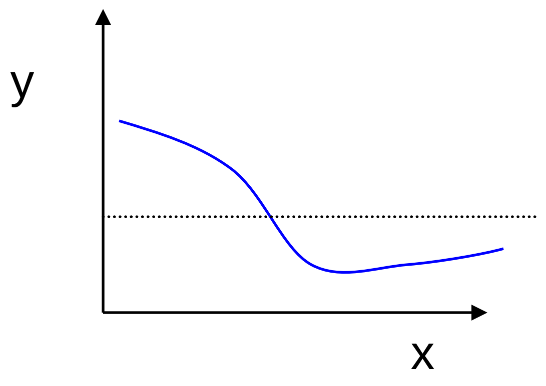
2. Perform polynomial Interpolation on the new table.

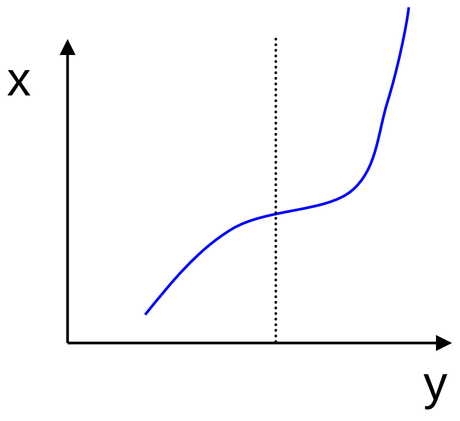
y_i	y_0	y_1	....	y_n
x_i	x_0	x_1	....	x_n

3. Evaluate

$$x = f_n(y_k)$$

Inverse Interpolation





Inverse Interpolation

Question:

What is the limitation of inverse interpolation?

- The original function has an inverse.
- $y_1, y_2, \ldots, y_n$ must be distinct.

Inverse Interpolation

Example

x	1	2	3
y	3.2	2.0	1.6

Problem :

Given the table. Find x such that $f(x) = 2.5$

3.2	1	-.8333	1.0417
2.0	2	-2.5	
1.6	3		

$$x = f_2(y) = 1 - 0.8333(y - 3.2) + 1.0417(y - 3.2)(y - 2)$$

$$x = f_2(2.5) = 1 - 0.8333(-0.7) + 1.0417(-0.7)(0.5) = 1.2187$$

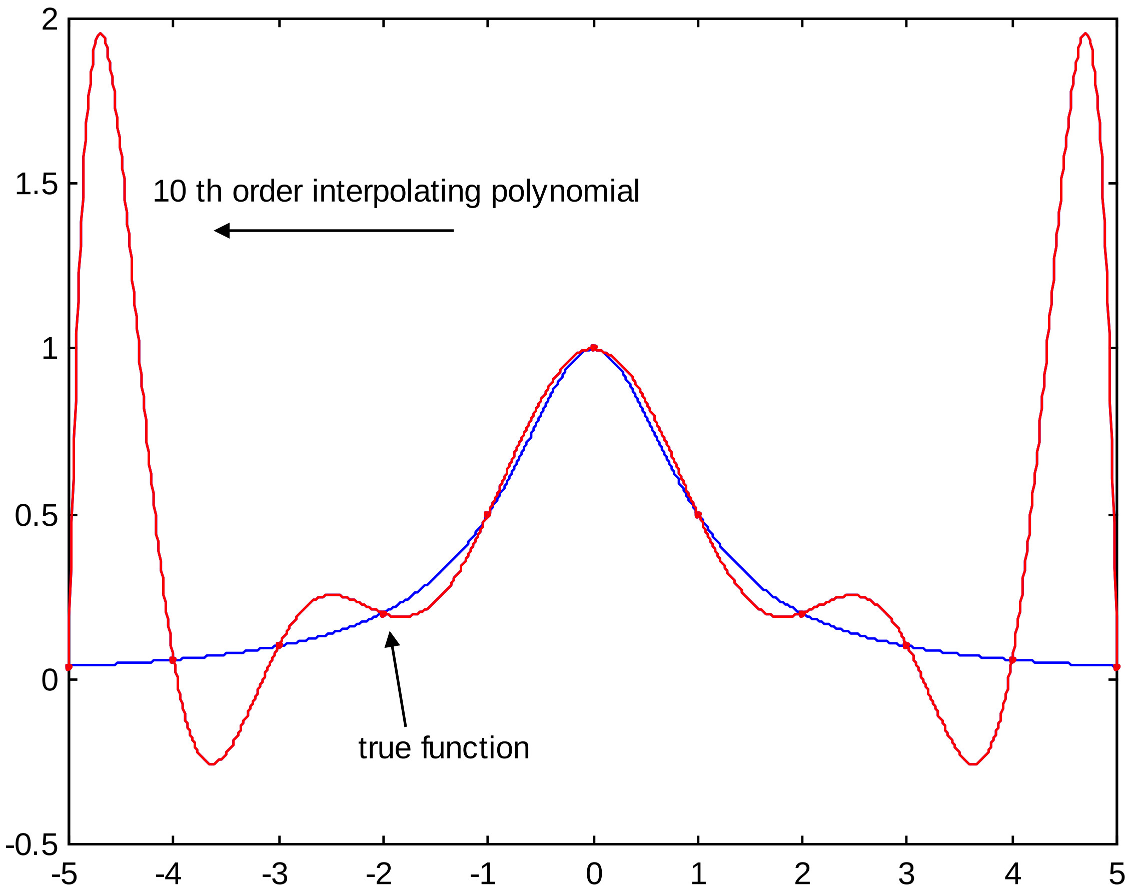
Errors in polynomial Interpolation

- Polynomial interpolation may lead to large errors (especially for high order polynomials).

BE CAREFUL

- When an n^{th} order interpolating polynomial is used, the error is related to the $(n+1)^{th}$ order derivative.

10^{th} Order Polynomial Interpolation



Errors in polynomial Interpolation

Theorem

Let $f(x)$ be a function such that:

$f^{(n+1)}(x)$ is continuous on [a, b], and $\left|f^{(n+1)}(x)\right| \leq M$.

Let $P(x)$ be any polynomial of degree $\leq$ n

that interpolates f at $n+1$ equally spaced points

in [a, b] (including the end points). Then:

$$\left|f(x)\text{-}P(x)\right| \leq \frac{M}{4(n+1)}\left(\frac{b-a}{n}\right)^{n+1}$$

Example

$f(x) = \sin(x)$

We want to use 9^{th} order polynomial to interpolate f(x) (using 10 equally spaced points) in the interval [0,1.6875].

$$\left| f^{(n+1)} \right| \leq 1 \quad for\ \ n > 0$$

$$M = 1,\ \ n = 9$$

$$\left| f(x)\text{-}P(x) \right| \leq \frac{M}{4(n+1)} \left(\frac{b-a}{n} \right)^{n+1}$$

$$\left| f(x)\text{-}P(x) \right| \leq \frac{1}{4(10)} \left(\frac{1.6875}{9} \right)^{10} = 1.34 \times 10^{-9}$$

Curve Fitting

What Is Curve Fitting?

- Data are often given for discrete values along a continuum. However, you may require estimates at points between the discrete values.
- One way to do this is to compute values of the function at a number of discrete values along the range of interest.
- Then, a simpler function may be derived to fit these values.
- Both of these applications are known as *curve fitting.*

Least Square Regression

- There are two general approaches for curve fitting that are distinguished from each other on the basis of the amount of error associated with the data.
- First, where the data exhibit a significant degree of error or "scatter" the strategy is to derive a single curve that represents the general trend of the data.
- Because any individual data point may be incorrect, we make no effort to intersect every point.
- Rather, the curve is designed to follow the pattern of the points taken as a group.
- One approach of this nature is called *least-squares regression*

Interpolation

- Second, where the data are known to be very precise, the basic approach is to fit a curve or a series of curves that pass directly through each of the points.
- Such data usually originate from tables.
- Examples are values for the density of water or for the heat capacity of gases as a function of temperature.
- The estimation of values between well-known discrete points is called *interpolation*

STATISTICS REVIEW

- mean,
- standard deviation,
- residual sum of the squares, and
- the normal distribution

Measure of Location

- The most common measure of central tendency is the arithmetic mean. The *arithmetic mean (Ý) of a sample is defined as the sum of the individual data* points *(yi) divided by the number of points (n), or*

$$\bar{y} = \frac{\sum y_i}{n}$$

where the summation (and all the succeeding summations in this section) is from *i = 1* through *n.*

Median

- The *median is the midpoint of a* group of data.
- It is calculated by first putting the data in ascending order.
- If the number of measurements is odd, the median is the middle value.
- If the number is even, it is the arithmetic mean of the two middle values.
- The median is sometimes called the *50th percentile.*

Mode

- The *mode is the value that occurs most frequently.*
- *The concept usually has direct utility* only when dealing with discrete or coarsely rounded data.

Measures of Spread

- The simplest measure of spread is the *range, the difference between* the largest and the smallest value.
- Although it is certainly easy to determine, it is not considered a very reliable measure because it is highly sensitive to the sample size and is very sensitive to extreme values.
- The most common measure of spread for a sample is the *standard deviation (sy) about* the mean:

$$s_y = \sqrt{\frac{S_t}{n-1}}$$

- where *St is the total sum of the squares of the residuals between the data points and the* mean, or

$$S_t = \sum (y_i - \bar{y})^2$$

variance

- The spread can also be represented by the square of the standard deviation, which is called the *variance:*

$$s_y^2 = \frac{\sum (y_i - \bar{y})^2}{n - 1}$$

- The quantity *n – 1* is referred to as the *degrees of freedom. Hence St and sy are said to be based on n – 1 degrees* of freedom

Example to solve

- Compute the mean, median, variance, standard deviation, and coefficient of variation for the data in Table

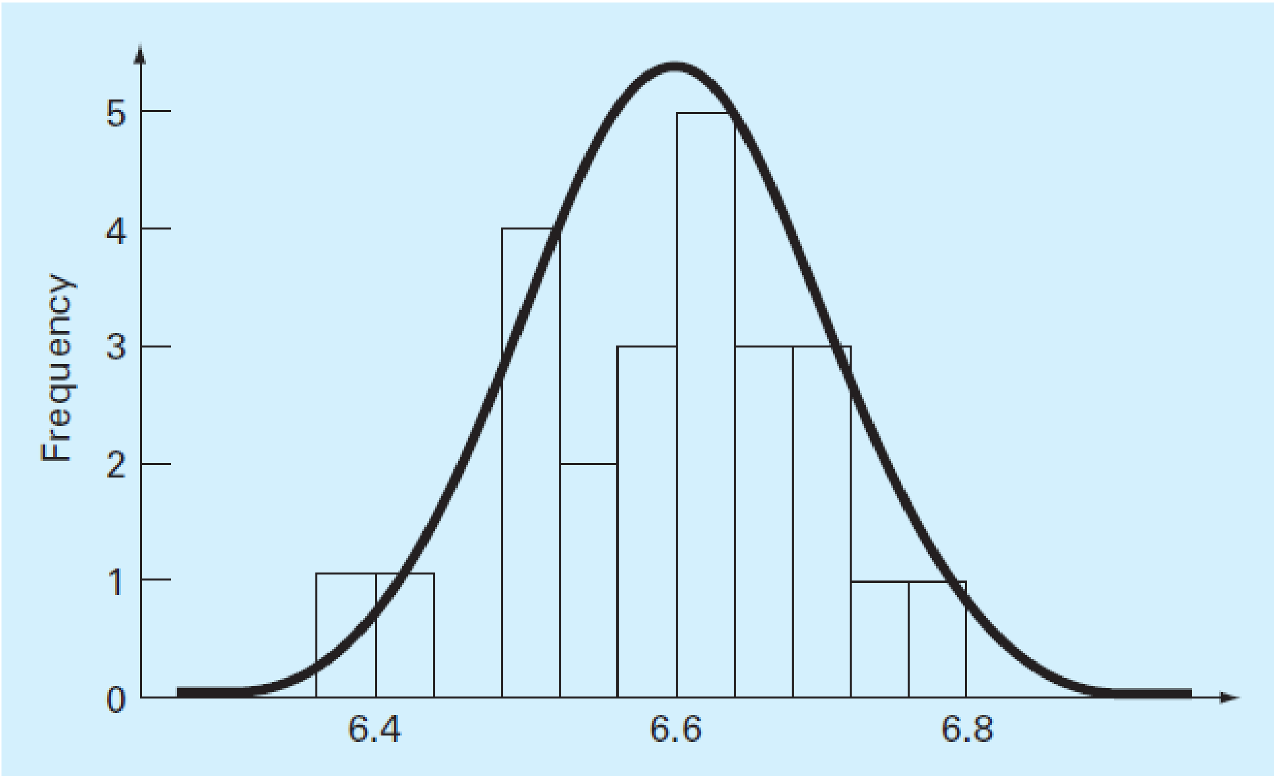
Measurements of the coefficient of thermal expansion of structural steel.

6.495	6.595	6.615	6.635	6.485	6.555
6.665	6.505	6.435	6.625	6.715	6.655
6.755	6.625	6.715	6.575	6.655	6.605
6.565	6.515	6.555	6.395	6.775	6.685

The Normal Distribution

- A histogram provides a simple visual representation of the distribution.
- A *histogram is constructed by sorting the measurements* into intervals, or *bins.*
- *The units of measurement are plotted on the abscissa and* the frequency of occurrence of each interval is plotted on the ordinate.
- If we have a very large set of data, the histogram often can be approximated by a smooth curve.
- The symmetric, bell-shaped curve is one such characteristic shape "the *normal distribution".*

Normal Distribution curve



Assignment

- If the initial velocity is zero, the downward velocity of the free-falling bungee jumper can be predicted with the following analytical solution

$$v = \sqrt{\frac{gm}{c_d}} \tanh\left(\sqrt{\frac{gc_d}{m}}\, t\right)$$

- Suppose that *g = 9.81m/s2, and m = 68.1 kg, but cd is not known precisely. For example,* you might know that it varies uniformly between 0.225 and 0*.275 (i.e., ±10%* around a mean value of 0.25 kg/m). Use the rand function to generate 1000 random uniformly distributed values of *cd and then employ these values along with the analytical solution to* compute the resulting distribution of velocities at *t = 4 s.*
- Analyze the same case as in Example, but rather than employing a uniform distribution, generate normally-distributed drag coefficients with a mean of 0.25 and a standard deviation of 0.01443.

LINEAR LEAST-SQUARES REGRESSION

- The mathematical expression for the straight line is

$$y = a_0 + a_1 x + e$$

- where *a0 and a1 are coefficients representing the intercept and the slope, respectively, and e is the error, or residual, between the model and the observations, which can be represented* by rearranging

$$e = y - a_0 - a_1 x$$

Criteria for a "Best" Fit

- One strategy for fitting a .best. line through the data would be to minimize the sum of the residual errors for all the available data, as in

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)$$

where *n = total number of points*

$$\sum_{i=1}^{n} |e_i| = \sum_{i=1}^{n} |y_i - a_0 - a_1 x_i|$$

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$$

This criterion, which is called *least squares.*

Least-Squares Fit of a Straight Line

- To determine values for *a0 and a1,equation is* differentiated with respect to each unknown coefficient:

$$\frac{\partial S_r}{\partial a_0} = -2\sum (y_i - a_0 - a_1 x_i)$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum [(y_i - a_0 - a_1 x_i)x_i]$$

- Note that we have simplified the summation symbols; unless otherwise indicated, all summations are from *i = 1 to n. Setting these derivatives equal to zero will result in a minimum Sr .*

- *If this is done, the equations can be expressed as*

$$0 = \sum y_i - \sum a_0 - \sum a_1 x_i$$

$$0 = \sum x_i y_i - \sum a_0 x_i - \sum a_1 x_i^2$$

- Now, realizing that ∑*a0 = na0, we can express the equations as a set of two simultaneous* linear equations with two unknowns (*a0 and a1):*

$$n \quad a_0 + \left(\sum x_i\right) a_1 = \sum y_i$$

$$\left(\sum x_i\right) a_0 + \left(\sum x_i^2\right) a_1 = \sum x_i y_i$$

- These are called the *normal equations.*

- They can be solved simultaneously for

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - \left(\sum x_i\right)^2}$$

- This result can then be used in conjunction with Eq. to solve for

$$a_0 = \bar{y} - a_1\bar{x}$$

- where $\bar{y}$ *and* $\bar{x}$ *are the means of y and x, respectively.*

Example to solve

- Fit a straight line to the values in the following table

v, m/s	10	20	30	40	50	60	70	80
F, N	25	70	380	550	610	1220	830	1450

Examples to solve

- Given the data

0.90	1.42	1.30	1.55	1.63
1.32	1.35	1.47	1.95	1.66
1.96	1.47	1.92	1.35	1.05
1.85	1.74	1.65	1.78	1.71
2.29	1.82	2.06	2.14	1.27

Determine (a) the mean, (b) median, (c) mode, (d) range, (e) standard deviation, (f) variance, and (g) coefficient of variation.

- Given the data

29.65	28.55	28.65	30.15	29.35	29.75	29.25
30.65	28.15	29.85	29.05	30.25	30.85	28.75
29.65	30.45	29.15	30.45	33.65	29.35	29.75
31.25	29.45	30.15	29.65	30.55	29.65	29.25

1. Determine (a) the mean, (b) median, (c) mode, (d) range, (e) standard deviation, (f) variance, and (g) coefficient of variation.
2. Construct a histogram. Use a range from 28 to 34 with increments of 0.4.

- Determine an equation to predict metabolism rate as a function of mass based on the following data. Use it to predict the metabolism rate of a 200-kg tiger.

Animal	Mass (kg)	Metabolism (watts)
Cow	400	270
Human	70	82
Sheep	45	50
Hen	2	4.8
Rat	0.3	1.45
Dove	0.16	0.97

POLYNOMIAL REGRESSION

POLYNOMIAL REGRESSION

- The least-squares procedure can be readily extended to fit the data to a higher-order polynomial. For example, suppose that we fit a second-order polynomial or quadratic:

$$y = a_0 + a_1 x + a_2 x^2 + e$$

- the sum of the squares of the residuals is

$$S_r = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - a_2 x_i^2 \right)^2$$

- To generate the least-squares fit, we take the derivative

$$\frac{\partial S_r}{\partial a_0} = -2\sum\left(y_i - a_0 - a_1 x_i - a_2 x_i^2\right)$$
$$\frac{\partial S_r}{\partial a_1} = -2\sum x_i\left(y_i - a_0 - a_1 x_i - a_2 x_i^2\right)$$
$$\frac{\partial S_r}{\partial a_2} = -2\sum x_i^2\left(y_i - a_0 - a_1 x_i - a_2 x_i^2\right)$$

set equal to zero and rearranged

$$(n)a_0 + \left(\sum x_i\right)a_1 + \left(\sum x_i^2\right)a_2 = \sum y_i$$
$$\left(\sum x_i\right)a_0 + \left(\sum x_i^2\right)a_1 + \left(\sum x_i^3\right)a_2 = \sum x_i y_i$$
$$\left(\sum x_i^2\right)a_0 + \left(\sum x_i^3\right)a_1 + \left(\sum x_i^4\right)a_2 = \sum x_i^2 y_i$$

- For this case, the standard error is formulated as

$$s_{y/x} = \sqrt{\frac{S_r}{n - (m + 1)}}$$

- This quantity is divided by *n − (m + 1) because (m + 1) data-derived coefficients. a0, a1, . . . , am.were used to compute Sr; thus, we have lost m + 1 degrees of freedom.*

Example

- Fit a second-order polynomial to the data in the following two columns

x_i	y_i
0	2.1
1	7.7
2	13.6
3	27.2
4	40.9
5	61.1
Σ	152.6

Error computation

x_i	y_i	$(y_i - \bar{y})^2$	$(y_i - a_0 - a_1 x_i - a_2 x_i^2)^2$
0	2.1	544.44	0.14332
1	7.7	314.47	1.00286
2	13.6	140.03	1.08160
3	27.2	3.12	0.80487
4	40.9	239.22	0.61959
5	61.1	1272.11	0.09434
Σ	152.6	2513.39	3.74657

$m = 2$ $\quad \sum x_i = 15$ $\quad \sum x_i^4 = 979$

$n = 6$ $\quad \sum y_i = 152.6$ $\quad \sum x_i y_i = 585.6$

$\bar{x} = 2.5$ $\quad \sum x_i^2 = 55$ $\quad \sum x_i^2 y_i = 2488.8$

$\bar{y} = 25.433$ $\quad \sum x_i^3 = 225$

Therefore, the simultaneous linear equations are

$$\begin{bmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 152.6 \\ 585.6 \\ 2488.8 \end{Bmatrix}$$

These equations can be solved to evaluate the coefficients. For example, using MATLAB:

```
>> N = [6 15 55;15 55 225;55 225 979];
>> r = [152.6 585.6 2488.8];
>> a = N\r

a =
     2.4786
     2.3593
     1.8607
```

Therefore, the least-squares quadratic equation for this case is

$$y = 2.4786 + 2.3593x + 1.8607x^2$$

The standard error of the estimate based on the regression polynomial is

$$s_{y/x} = \sqrt{\frac{3.74657}{6-(2+1)}} = 1.1175$$

The coefficient of determination is

$$r^2 = \frac{2513.39 - 3.74657}{2513.39} = 0.99851$$

and the correlation coefficient is $r = 0.99925$.

Practice problem

1. Fit a cubic polynomial to the following data

x	3	4	5	7	8	9	11	12
y	1.6	3.6	4.4	3.4	2.2	2.8	3.8	4.6

Along with the coefficients, determine *r 2 and sy/x* .

Numerical Differentiation

What Is Differentiation?

- *Calculus is the mathematics of change.*
- *Because engineers and scientists must continuously* deal with systems and processes that change, calculus is an essential tool of our profession.
- Standing at the heart of calculus is the mathematical concept of differentiation.
- According to the dictionary definition, to *differentiate means .to mark off by differences;* distinguish; . . . to perceive the difference in or between..
- Mathematically, the *derivative,* which serves as the fundamental vehicle for differentiation, represents the rate of change of a dependent variable with respect to an independent variable.

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

Practical Example

- How do you evaluate the derivative of a tabulated function.
- How do we determine the velocity and acceleration from tabulated measurements.

Time (second)	Displacement (meters)
0	30.1
5	48.2
10	50.0
15	40.2

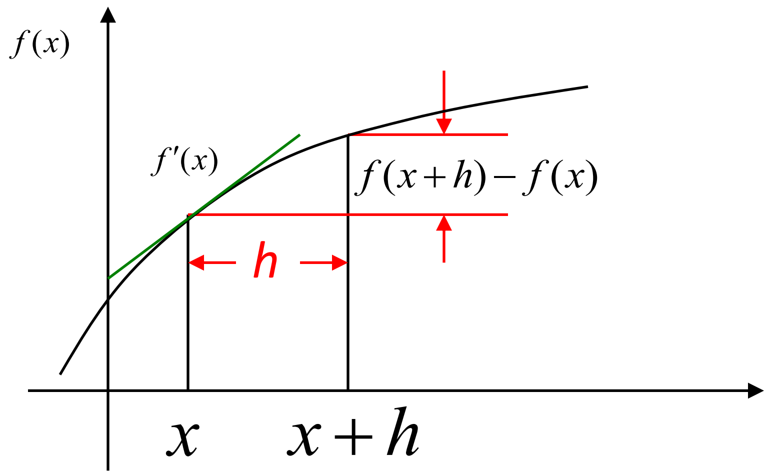
Three approaches

- Methods based on interpolation
- Methods based on difference operators
  - Forward difference
  - Backward difference
  - Center difference
- Methods based on undetermined coefficients

Forward Difference Formula for $f'(x)$

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \qquad error = O(h)$$

Geometrically



Backward Difference Formula for $f'(x)$

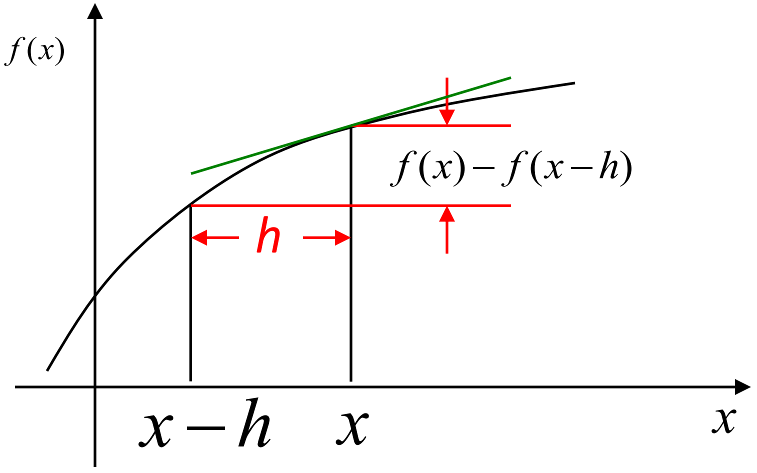
Similarly

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2} f''(x)h^2 + O(h^3)$$

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

$$error = O(h)$$

Geometrically



Central Difference Formula for $f'(x)$

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(x)h^3 + \frac{1}{4!}f^{(4)}(x)h^4 + O(h^5)$$

$$-)\quad f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(x)h^3 + \frac{1}{4!}f^{(4)}(x)h^4 + O(h^5)$$

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{1}{3}f'''(x)h^3 + O(h^5)$$

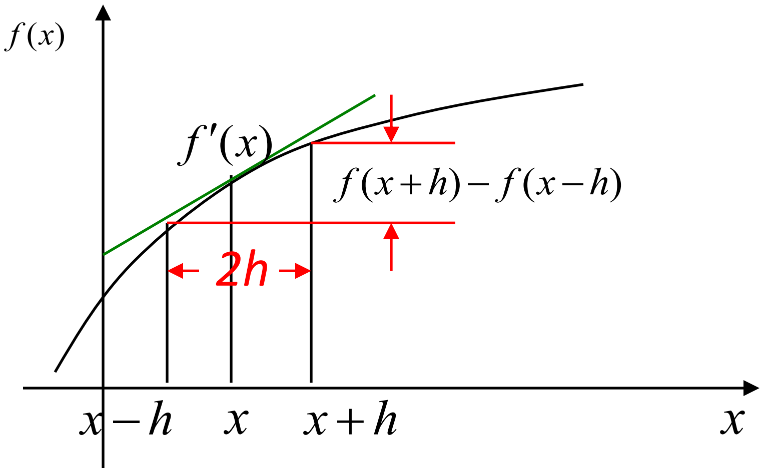
$$2hf'(x) = f(x+h) - f(x-h) - \frac{1}{3}f'''(x)h^3 + O(h^5)$$

Central Difference Formula for $f'(x)$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

$$error = O(h^2)$$

Geometrically



Example

$$\left[\frac{d}{dx}\tan^{-1}(x)\right]_{x=1}$$

$$\frac{\tan^{-1}\left(1+10^{-4}\right)-\tan^{-1}(1)}{10^{-4}}$$

ε = 5e-5

$$\frac{\tan^{-1}\left(1+10^{-4}\right)-\tan^{-1}\left(1-10^{-4}\right)}{2\times 10^{-4}}$$

ε = 2e-9

$$\frac{\tan^{-1}(1)-\tan^{-1}\left(1-10^{-4}\right)}{10^{-4}}$$

ε = 5e-5

The Three Formula (Revisited)

Forward Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h} + O(h)$$

Backward Difference: $$\frac{df(x)}{dx} = \frac{f(x) - f(x-h)}{h} + O(h)$$

Central Difference : $$\frac{df(x)}{dx} = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

Forward and backward difference formulas are comparable in accuracy.

Central difference formula is expected to give a better answer.

Higher Order Formulas

$$f(x+h) = f(x) + f'(x)h + \frac{f^{(2)}(x)h^2}{2!} + \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f^{(2)}(x)h^2}{2!} - \frac{f^{(3)}(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$f(x+h) + f(x-h) = 2f(x) + 2\frac{f^{(2)}(x)h^2}{2!} + 2\frac{f^{(4)}(x)h^4}{4!} + \ldots$$

$$\Rightarrow \; f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$

$$\boxed{Error = -\frac{f^{(4)}(\xi)h^2}{12}}$$

Other Higher Order Formulas

$$f^{(2)}(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

$$f^{(3)}(x) = \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{2h^3}$$

$$f^{(4)}(x) = \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4}$$

Central Formulas with $Error = O(h^2)$

Other formulas for $f^{(2)}(x), f^{(3)}(x)$... are also possible.

You can use Taylor Theorem to prove them and obtain the error order.

Example

- Use forward, backward and centered difference approximations to estimate the first derivate of:

  $f(x) = –0.1x^4 – 0.15x^3 – 0.5x^2 – 0.25x + 1.2$

  at $x = 0.5$ using step size $h = 0.5$ and $h = 0.25$

- Note that the derivate can be obtained directly:

  $f'(x) = –0.4x^3 – 0.45x^2 – 1.0x – 0.25$

  The true value of $f'(0.5) = -0.9125$

- In this example, the function and its derivate are known. However, in general, only tabulated data might be given.

Solution with Step Size = 0.5

- f(0.5) = 0.925, f(0) = 1.2, f(1.0) = 0.2
- Forward Divided Difference:

  $f'(0.5) \approx (0.2 - 0.925)/0.5 = -1.45$

  $|\varepsilon_t| = |(-0.9125+1.45)/-0.9125| = 58.9\%$
- Backward Divided Difference:

  $f'(0.5) \approx (0.925 - 1.2)/0.5 = -0.55$

  $|\varepsilon_t| = |(-0.9125+0.55)/-0.9125| = 39.7\%$
- Centered Divided Difference:

  $f'(0.5) \approx (0.2 - 1.2)/1.0 = -1.0$

  $|\varepsilon_t| = |(-0.9125+1.0)/-0.9125| = 9.6\%$

Solution with Step Size = 0.25

- f(0.5)=0.925, f(0.25)=1.1035, f(0.75)=0.6363
- Forward Divided Difference:

  f'(0.5) ≈ (0.6363 – 0.925)/0.25 = -1.155

  $|\varepsilon_t|$ = |(-0.9125+1.155)/-0.9125| = 26.5%
- Backward Divided Difference:

  f'(0.5) ≈ (0.925 – 1.1035)/0.25 = -0.714

  $|\varepsilon_t|$ = |(-0.9125+0.714)/-0.9125| = 21.7%
- Centered Divided Difference:

  f'(0.5) ≈ (0.6363 – 1.1035)/0.5 = -0.934

  $|\varepsilon_t|$ = |(-0.9125+0.934)/-0.9125| = 2.4%

Discussion

- For both the Forward and Backward difference, the error is O(h)
- Halving the step size h approximately halves the error of the Forward and Backward differences
- The Centered difference approximation is more accurate than the Forward and Backward differences because the error is $O(h^2)$
- Halving the step size h approximately quarters the error of the Centered difference.

Example 2

Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, $h = 0.05$, and $h = 0.01$, and determine bounds for the approximation errors.

Solution

The forward-difference formula

$$\frac{f(1.8 + h) - f(1.8)}{h}$$

with $h = 0.1$ gives

$(\ln 1.9 - \ln 1.8)/0.1$

$= (0.64185389 - 0.58778667)/0.1 = 0.5406722.$

Because $f''(x) = -1/x^2$ and $1.8 < \xi < 1.9$, a bound for this approximation error is $|hf''(\xi)|/2$

$= |h|/2\xi^2 < 0.1/2(1.8)^2 = 0.0154321.$

h	$f(1.8+h)$	$\dfrac{f(1.8+h)-f(1.8)}{h}$	$\dfrac{\lvert h\rvert}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

NUMERICAL INTEGRATION

What is Integration

Integration:

The process of measuring the area under a function plotted on a graph.

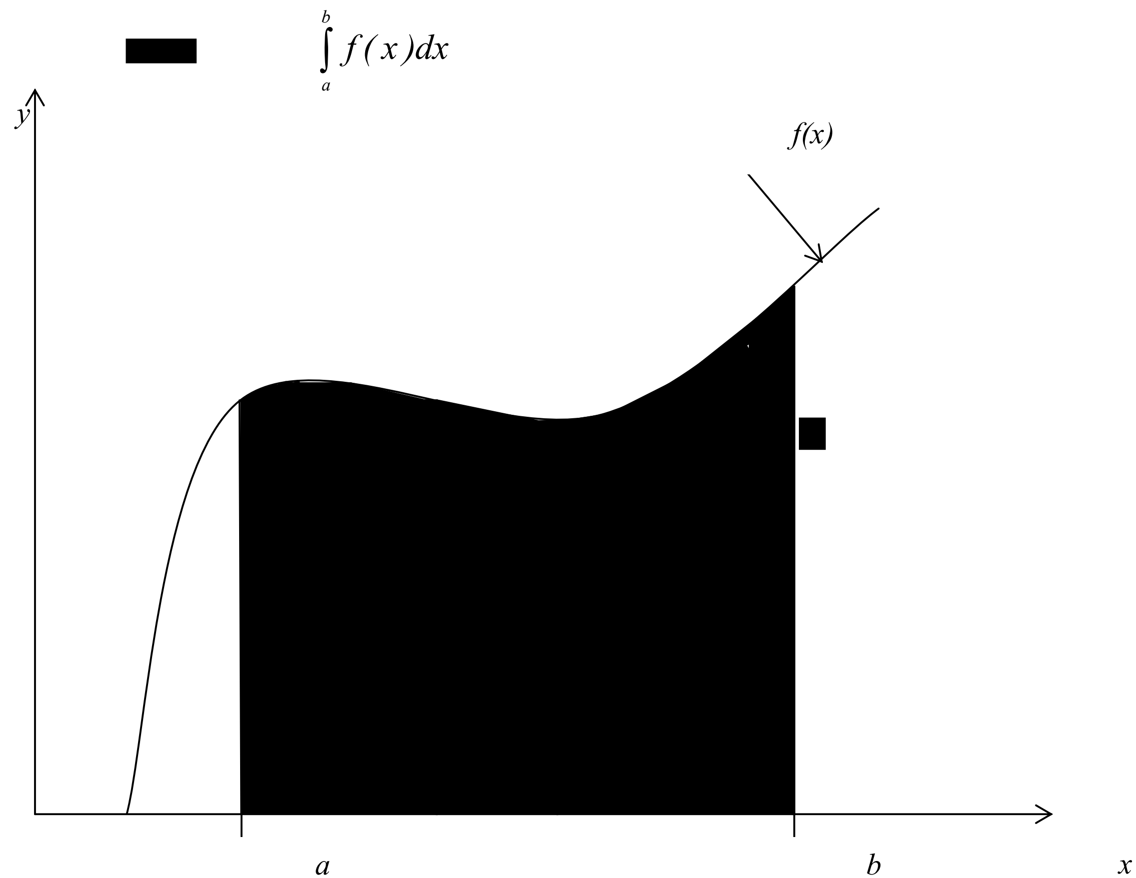
$$I = \int_a^b f(x)\,dx$$

Where:

f(x) is the integrand

a= lower limit of integration

b= upper limit of integration



Method Derived From Geometry

The area under the curve is a trapezoid. The integral

$$\int_a^b f(x)dx \approx Area\ of\ \ trapezoid$$

$$= \frac{1}{2}(Sum\ of\ parallel\ sides)(height)$$

$$= \frac{1}{2}\left(f(b)+f(a)\right)(b-a)$$

$$= (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

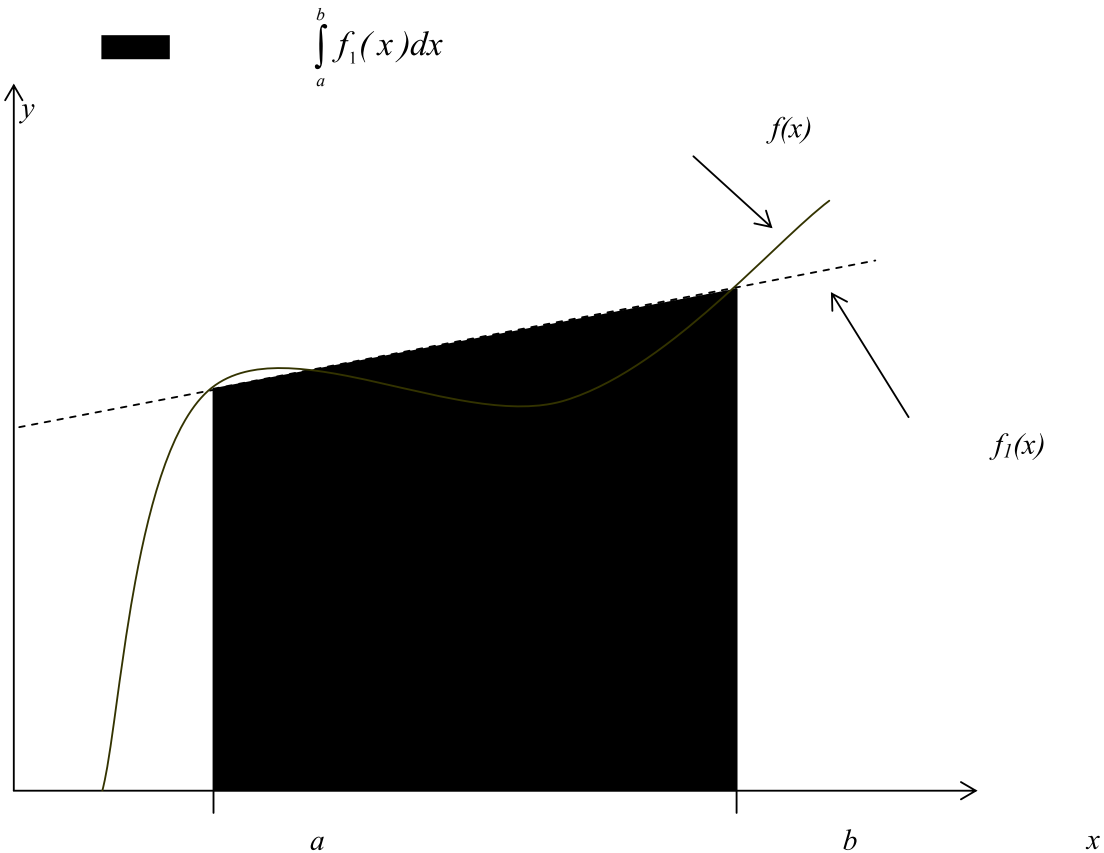


Figure 2: Geometric Representation

Example 1

The vertical distance covered by a rocket from t=8 to t=30 seconds is given by:

$$x = \int_{8}^{30} \left(2000 ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use single segment Trapezoidal rule to find the distance covered.
b) Find the true error, E_t for part (a).
c) Find the absolute relative true error, $|\epsilon_a|$ for part (a).

Solution

a) $$I \approx (b-a)\left[\frac{f(a)+f(b)}{2}\right]$$

$$a = 8 \qquad b = 30$$

$$f(t) = 2000 ln\left[\frac{140000}{140000-2100t}\right] - 9.8t$$

$$f(8) = 2000 ln\left[\frac{140000}{140000-2100(8)}\right] - 9.8(8) \qquad = 177.27\ m/s$$

$$f(30) = 2000 ln\left[\frac{140000}{140000-2100(30)}\right] - 9.8(30) \quad = 901.67\ m/s$$

Solution (cont)

a) $$I = (30-8)\left[\frac{177.27+901.67}{2}\right]$$

$$=11868\, m$$

b) The exact value of the above integral is

$$x = \int_{8}^{30}\left(2000 ln\left[\frac{140000}{140000-2100t}\right]-9.8t\right)dt \quad =11061\, m$$

Solution (cont)

b)

$$E_t = True\ Value - Approximate\ Value$$

$$= 11061 - 11868$$

$$= -807\ m$$

c) The absolute relative true error, $\left|\in_t\right|$, would be

$$\left|\in_t\right| = \left|\frac{11061 - 11868}{11061}\right| \times 100 = 7.2959\%$$

Multiple Segment Trapezoidal Rule

In Example 1, the true error using single segment trapezoidal rule was large. We can divide the interval [8,30] into [8,19] and [19,30] intervals and apply Trapezoidal rule over each segment.

$$f(t) = 2000 \ln\left(\frac{140000}{140000 - 2100t}\right) - 9.8t$$

$$\int_{8}^{30} f(t)dt = \int_{8}^{19} f(t)dt + \int_{19}^{30} f(t)dt$$

$$= (19-8)\left[\frac{f(8)+f(19)}{2}\right] + (30-19)\left[\frac{f(19)+f(30)}{2}\right]$$

Multiple Segment Trapezoidal Rule

With

$$f(8) = 177.27\ m/s$$

$$f(30) = 901.67\ m/s$$

$$f(19) = 484.75\ m/s$$

Hence:

$$\int_{8}^{30} f(t)dt = (19-8)\left[\frac{177.27+484.75}{2}\right] + (30-19)\left[\frac{484.75+901.67}{2}\right]$$

$$= 11266\ m$$

Multiple Segment Trapezoidal Rule

The true error is:

$$E_t = 11061 - 11266$$
$$= -205\ m$$

The true error now is reduced from -807 m to -205 m.

Extending this procedure to divide the interval into equal segments to apply the Trapezoidal rule; the sum of the results obtained for each segment is the approximate value of the integral.

Multiple Segment Trapezoidal Rule

Divide into equal segments as shown in Figure 4. Then the width of each segment is:

$$h = \frac{b-a}{n}$$

The integral I is:

$$I = \int_{a}^{b} f(x)dx$$

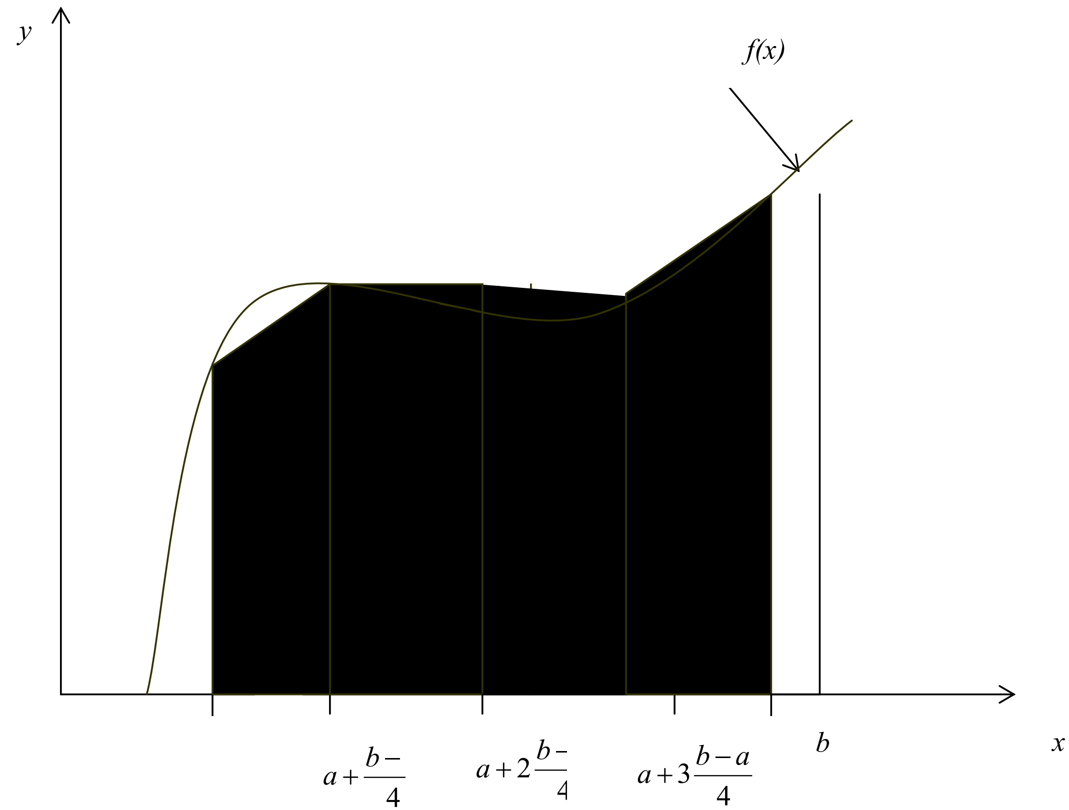


Figure 4: Multiple (n=4) Segment Trapezoidal Rule

Multiple Segment Trapezoidal Rule

The integral *I* can be broken into *h* integrals as:

$$\int_a^b f(x)dx = \int_a^{a+h} f(x)dx + \int_{a+h}^{a+2h} f(x)dx + \ldots + \int_{a+(n-2)h}^{a+(n-1)h} f(x)dx + \int_{a+(n-1)h}^{b} f(x)dx$$

Applying Trapezoidal rule on each segment gives:

$$\int_a^b f(x)dx = \frac{b-a}{2n}\left[f(a)+2\left\{\sum_{i=1}^{n-1} f(a+ih)\right\}+f(b)\right]$$

Simpson's 1/3rd Rule

Basis of Simpson's 1/3rd Rule

Trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating the polynomial in the interval of integration. Simpson's 1/3rd rule is an extension of Trapezoidal rule where the integrand is approximated by a second order polynomial.

Hence

$$I = \int_a^b f(x)dx \approx \int_a^b f_2(x)dx$$

Where $f_2(x)$ is a second order polynomial.

$$f_2(x) = a_0 + a_1 x + a_2 x^2$$

Basis of Simpson's 1/3rd Rule

Choose

$$(a, f(a)),\ \left(\frac{a+b}{2}, f\left(\frac{a+b}{2}\right)\right), \quad \text{and} \quad (b, f(b))$$

as the three points of the function to evaluate a_0, a_1 and a_2.

$$f(a) = f_2(a) = a_0 + a_1 a + a_2 a^2$$

$$f\left(\frac{a+b}{2}\right) = f_2\left(\frac{a+b}{2}\right) = a_0 + a_1\left(\frac{a+b}{2}\right) + a_2\left(\frac{a+b}{2}\right)^2$$

$$f(b) = f_2(b) = a_0 + a_1 b + a_2 b^2$$

Basis of Simpson's 1/3rd Rule

Solving the previous equations for a_0, a_1 and a_2 give

$$a_0 = \frac{a^2 f(b) + abf(b) - 4abf\left(\frac{a+b}{2}\right) + abf(a) + b^2 f(a)}{a^2 - 2ab + b^2}$$

$$a_1 = -\frac{af(a) - 4af\left(\frac{a+b}{2}\right) + 3af(b) + 3bf(a) - 4bf\left(\frac{a+b}{2}\right) + bf(b)}{a^2 - 2ab + b^2}$$

$$a_2 = \frac{2\left(f(a) - 2f\left(\frac{a+b}{2}\right) + f(b)\right)}{a^2 - 2ab + b^2}$$

Basis of Simpson's 1/3rd Rule

Then

$$I \approx \int_a^b f_2(x)dx$$

$$= \int_a^b \left(a_0 + a_1 x + a_2 x^2\right)dx$$

$$= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3}\right]_a^b$$

$$= a_0(b-a) + a_1 \frac{b^2 - a^2}{2} + a_2 \frac{b^3 - a^3}{3}$$

Basis of Simpson's 1/3rd Rule

Substituting values of a_0, a_1, a_2 give

$$\int_a^b f_2(x)dx = \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

Since for Simpson's 1/3rd Rule, the interval [a, b] is broken

into 2 segments, the segment width

$$h = \frac{b-a}{2}$$

Basis of Simpson's 1/3rd Rule

Hence

$$\int_a^b f_2(x)dx = \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

Because the above form has 1/3 in its formula, it is called Simpson's 1/3rd Rule.

Example 1

The distance covered by a rocket from t=8 to t=30 is given by

$$x = \int_{8}^{30} \left(2000\, ln\left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use Simpson's 1/3rd Rule to find the approximate value of x

b) Find the true error, E_t

c) Find the absolute relative true error, $|\in_t|$

Solution

a)

$$x = \int_{8}^{30} f(t)dt$$

$$x = \left(\frac{b-a}{6}\right)\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

$$= \left(\frac{30-8}{6}\right)[f(8) + 4f(19) + f(30)]$$

$$= \left(\frac{22}{6}\right)[177.2667 + 4(484.7455) + 901.6740]$$

$$= 11065.72\ m$$

Solution (cont)

b) The exact value of the above integral is

$$x = \int_{8}^{30} \left(2000\, ln\left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

$$= 11061.34\ m$$

True Error

$$E_t = 11061.34 - 11065.72$$

$$= -4.38\ m$$

Solution (cont)

a)c) Absolute relative true error,

$$\left|\in_t\right| = \left|\frac{11061.34 - 11065.72}{11061.34}\right| \times 100\%$$

$$= 0.0396\%$$

Multiple Segment Simpson's 1/3rd Rule

Multiple Segment Simpson's 1/3rd Rule

Just like in multiple segment Trapezoidal Rule, one can subdivide the interval

[a, b] into n segments and apply Simpson's 1/3rd Rule repeatedly over

every two segments. Note that n needs to be even. Divide interval

[a, b] into equal segments, hence the segment width

$$h = \frac{b-a}{n} \qquad \int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx$$

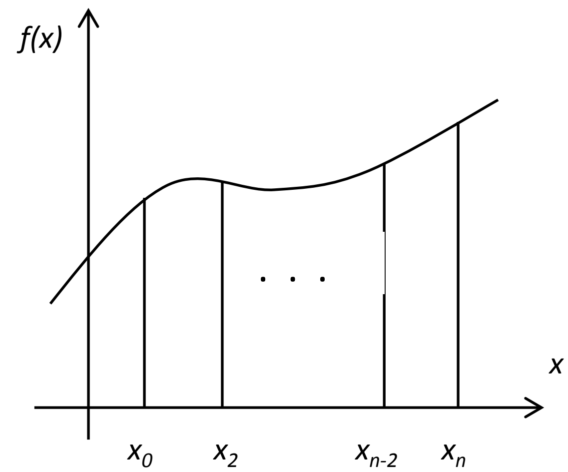
where

$$x_0 = a \qquad x_n = b$$

Multiple Segment Simpson's 1/3rd Rule

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \ldots\ldots$$

$$\ldots\ldots + \int_{x_{n-4}}^{x_{n-2}} f(x)dx + \int_{x_{n-2}}^{x_n} f(x)dx$$



Apply Simpson's 1/3rd Rule over each interval,

$$\int_a^b f(x)dx = (x_2 - x_0)\left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}\right] + \ldots$$

$$+ (x_4 - x_2)\left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6}\right] + \ldots$$

Multiple Segment Simpson's 1/3rd Rule

$$\ldots+(x_{n-2}-x_{n-4})\left[\frac{f(x_{n-4})+4f(x_{n-3})+f(x_{n-2})}{6}\right]+\ldots$$

$$+(x_n-x_{n-2})\left[\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}\right]$$

Since

$$x_i-x_{i-2}=2h \qquad\qquad i=2,\ 4,\ \ldots,\ n$$

Multiple Segment Simpson's 1/3rd Rule

Then

$$\int_a^b f(x)dx = 2h\left[\frac{f(x_0)+4f(x_1)+f(x_2)}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_2)+4f(x_3)+f(x_4)}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_{n-4})+4f(x_{n-3})+f(x_{n-2})}{6}\right]+\ldots$$

$$+2h\left[\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}\right]$$

Multiple Segment Simpson's 1/3rd Rule

$$\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0)+4\{f(x_1)+f(x_3)+\ldots+f(x_{n-1})\}+\ldots\right]$$

$$\ldots+2\{f(x_2)+f(x_4)+\ldots+f(x_{n-2})\}+f(x_n)\}]$$

$$=\frac{h}{3}\left[f(x_0)+4\sum_{\substack{i=1\\ i=odd}}^{n-1}f(x_i)+2\sum_{\substack{i=2\\ i=even}}^{n-2}f(x_i)+f(x_n)\right]$$

$$=\frac{b-a}{3n}\left[f(x_0)+4\sum_{\substack{i=1\\ i=odd}}^{n-1}f(x_i)+2\sum_{\substack{i=2\\ i=even}}^{n-2}f(x_i)+f(x_n)\right]$$

Example 2

Use 4-segment Simpson's 1/3rd Rule to approximate the distance

covered by a rocket from t= 8 to t=30 as given by

$$x = \int_{8}^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use four segment Simpson's 1/3rd Rule to find the approximate value of *x*.
b) Find the true error, E_t for part (a).
c) Find the absolute relative true error, $|\epsilon_a|$ for part (a).

Solution

a) Using n segment Simpson's 1/3rd Rule,

$$h=\frac{30-8}{4}=5.5$$

So

$$f(t_0)=f(8)$$

$$f(t_1)=f(8+5.5)=f(13.5)$$

$$f(t_2)=f(13.5+5.5)=f(19)$$

$$f(t_3)=f(19+5.5)=f(24.5)$$

$$f(t_4)=f(30)$$

Solution (cont.)

$$x = \frac{b-a}{3n}\left[f(t_0) + 4\sum_{\substack{i=1 \\ i=odd}}^{n-1} f(t_i) + 2\sum_{\substack{i=2 \\ i=even}}^{n-2} f(t_i) + f(t_n) \right]$$

$$= \frac{30-8}{3(4)}\left[f(8) + 4\sum_{\substack{i=1 \\ i=odd}}^{3} f(t_i) + 2\sum_{\substack{i=2 \\ i=even}}^{2} f(t_i) + f(30) \right]$$

$$= \frac{22}{12}\left[f(8) + 4f(t_1) + 4f(t_3) + 2f(t_2) + f(30) \right]$$

Solution (cont.)

cont.

$$=\frac{11}{6}\left[f(8)+4f(13.5)+4f(24.5)+2f(19)+f(30)\right]$$

$$=\frac{11}{6}\left[177.2667+4(320.2469)+4(676.0501)+2(484.7455)+901.6740\right]$$

$$=11061.64\ m$$

Solution (cont.)

b) In this case, the true error is

$$E_t = 11061.34 - 11061.64 = -0.30\ m$$

c) The absolute relative true error

$$\left|\in_t\right| = \left|\frac{11061.34 - 11061.64}{11061.34}\right| \times 100\%$$

$$= 0.0027\%$$

Solution (cont.)

Table 1: Values of Simpson's 1/3rd Rule for Example 2 with multiple segments

n	Approximate Value	E_t	$\|\epsilon_t\|$
2	11065.72	4.38	0.0396%
4	11061.64	0.30	0.0027%
6	11061.40	0.06	0.0005%
8	11061.35	0.01	0.0001%
10	11061.34	0.00	0.0000%

Tutorial

Use the trapezoidal rule to numerically integrate

$$f(x) = 0.2 + 25x$$

Use the trapezoidal rule to numerically integrate

$$f(x) = 0.2 + 25x + 3x^2$$

Use Simpson's 1/3 rule to integrate

$$f(x) = 0.2 + 25x + 3x^2 + 8x^3$$

Use Simpson's 1/3 rule to integrate

$$f(x) = 0.2 + 25x + 3x^2 + 2x^4$$

ODE Solver

EULER’S METHOD

Euler's Method

$$\frac{dy}{dx} = f(x,y), y(0) = y_0$$

Slope $= \dfrac{Rise}{Run}$

$$= \frac{y_1 - y_0}{x_1 - x_0}$$

$$= f(x_0, y_0)$$

$$y_1 = y_0 + f(x_0, y_0)(x_1 - x_0)$$
$$= y_0 + f(x_0, y_0)h$$

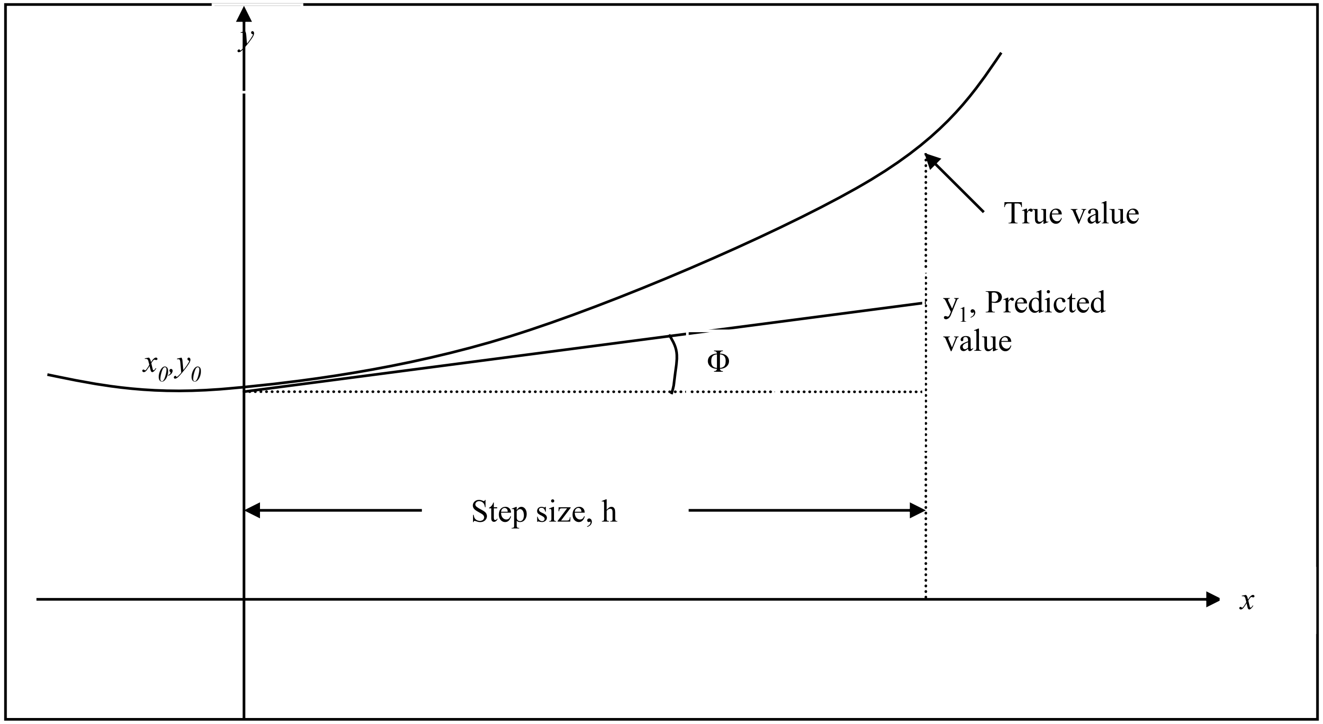


Figure 1 Graphical interpretation of the first step of Euler's method

Euler's Method

$$y_{i+1} = y_i + f(x_i, y_i)h$$

$$h = x_{i+1} - x_i$$

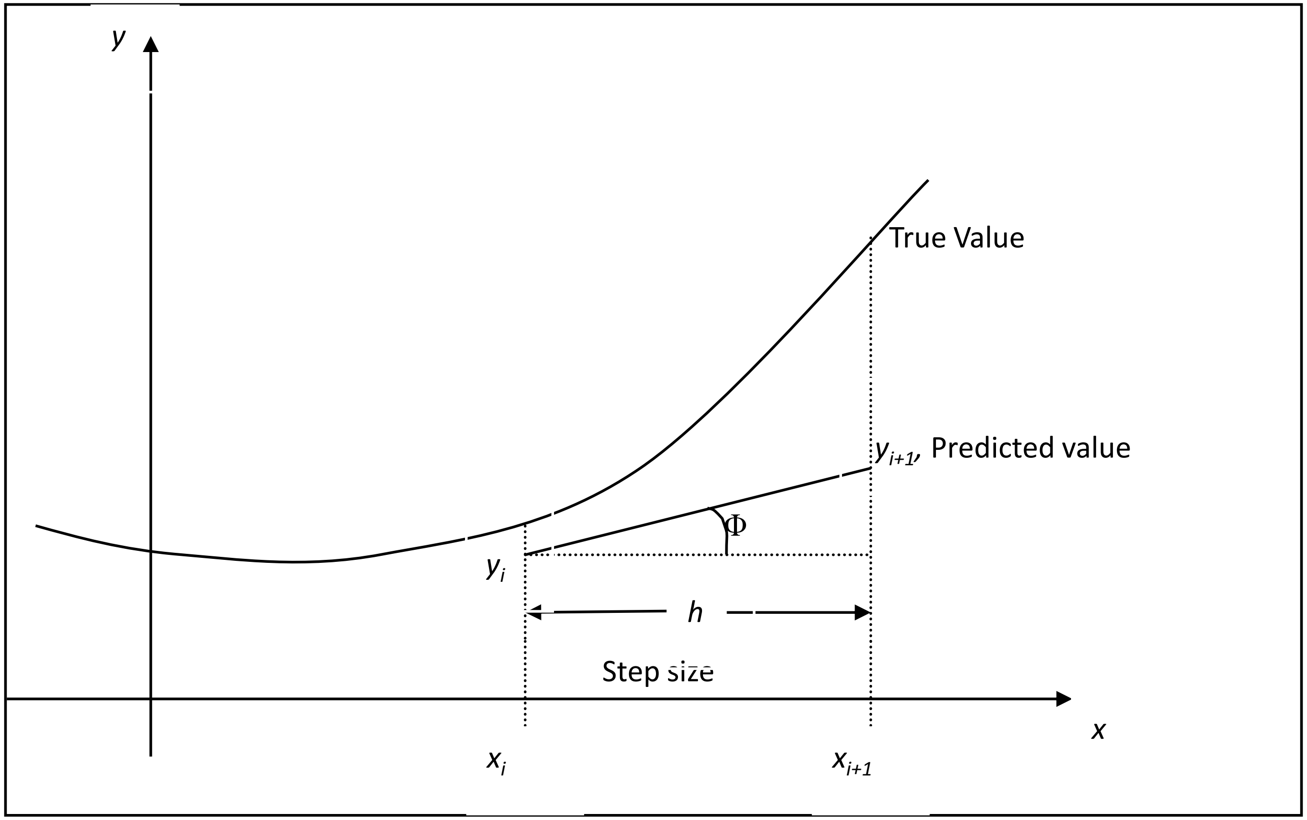


Figure 2. General graphical interpretation of Euler's method

How to write Ordinary Differential Equation

How does one write a first order differential equation in the form of

$$\frac{dy}{dx} = f(x, y)$$

Example

$$\frac{dy}{dx} + 2y = 1.3e^{-x}, y(0) = 5$$

is rewritten as

$$\frac{dy}{dx} = 1.3e^{-x} - 2y, y(0) = 5$$

In this case

$$f(x, y) = 1.3e^{-x} - 2y$$

Example

A ball at 1200K is allowed to cool down in air at an ambient temperature of 300K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right), \theta(0) = 1200K$$

Find the temperature at $t = 480$ seconds using Euler's method. Assume a step size of $h = 240$ seconds.

Solution

Step 1:

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$f(t,\theta) = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$\theta_{i+1} = \theta_i + f(t_i,\theta_i)h$$

$$\begin{aligned}\theta_1 &= \theta_0 + f(t_0,\theta_0)h \\ &= 1200 + f(0,1200)240 \\ &= 1200 + \left(-2.2067\times10^{-12}\left(1200^4 - 81\times10^8\right)\right)240 \\ &= 1200 + (-4.5579)240 \\ &= 106.09K\end{aligned}$$

θ_1 is the approximate temperature at $t = t_1 = t_0 + h = 0 + 240 = 240$

$$\theta(240) \approx \theta_1 = 106.09K$$

Solution Cont

Step 2: For $i = 1, \quad t_1 = 240, \quad \theta_1 = 106.09$

$$
\begin{aligned}
\theta_2 &= \theta_1 + f(t_1, \theta_1)h \\
&= 106.09 + f(240, 106.09)240 \\
&= 106.09 + \left(-2.2067 \times 10^{-12}\left(106.09^4 - 81 \times 10^8\right)\right)240 \\
&= 106.09 + (0.017595)240 \\
&= 110.32K
\end{aligned}
$$

θ_2 is the approximate temperature at $t = t_2 = t_1 + h = 240 + 240 = 480$

$$\theta(480) \approx \theta_2 = 110.32K$$

Solution Cont

The exact solution of the ordinary differential equation is given by the solution of a non-linear equation as

$$0.92593\ln\frac{\theta-300}{\theta+300}-1.8519\tan^{-1}(0.00333\theta)=-0.22067\times10^{-3}t-2.9282$$

The solution to this nonlinear equation at t=480 seconds is

$$\theta(480)=647.57K$$

RK METHOD

Runge-Kutta 2nd Order Method

For $\dfrac{dy}{dx} = f(x, y), y(0) = y_0$

Runge Kutta 2nd order method is given by

$$y_{i+1} = y_i + \left(a_1 k_1 + a_2 k_2\right)h$$

where

$$k_1 = f\left(x_i, y_i\right)$$

$$k_2 = f\left(x_i + p_1 h, y_i + q_{11} k_1 h\right)$$

Example

A polluted lake with an initial concentration of a bacteria is 10^7 parts/m^3, while the acceptable level is only 5×10^6 parts/m^3. The concentration of the bacteria will reduce as fresh water enters the lake. The differential equation that governs the concentration *C* of the pollutant as a function of time (in weeks) is given by

$$\frac{dC}{dt} + 0.06C = 0, C(0) = 10^7$$

Find the concentration of the pollutant after 7 weeks. Take a step size of 3.5 weeks.

$$\frac{dC}{dt} = -0.06C$$

$$f(t, C) = -0.06C$$

$$C_{i+1} = C_i + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h$$

Solution

Step 1: $i = 0,\ t_0 = 0,\ C_0 = 10^7$

$$k_1 = f(t_0, C_0) = f(0, 10^7) = -0.06(10^7) = -600000$$

$$k_2 = f(t_0 + h,\ C_0 + k_1 h) = f(0 + 3.5,\ 10^7 + (-600000)3.5)$$
$$= f(3.5,\ 7.9 \times 10^6) = -0.06(7.9 \times 10^6) = -474000$$

$$C_1 = C_0 + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h$$
$$= 10^7 + \left(\frac{1}{2}(-600000) + \frac{1}{2}(-474000)\right)3.5$$
$$= 10^7 + (-537000)3.5$$
$$= 8.1205 \times 10^6 \text{ parts/m}^3$$

C_1 is the approximate concentration of bacteria at

$$t = t_1 = t_0 + h = 0 + 3.5 = 3.5 \text{ weeks}$$

$$C(3.5) \approx C_1 = 8.1205 \times 10^6 \text{ parts/m}^3$$

Solution Cont

Step 2: $i=1,\ t_1=t_0+h=0+3.5=3.5,\ \ C_1=8.1205\times10^6\,\text{parts/m}^3$

$$k_1=f(t_1,C_1)=f\left(3.5,\ 8.1205\times10^6\right)=-0.06\left(8.1205\times10^6\right)=-487230$$

$$k_2=f(t_1+h,C_1+k_1h)=f\left(3.5+3.5,\ 8.1205\times10^6+(-487230)3.5\right)$$
$$=f(7,\ 6415200)=-0.06(6415200)=-384910$$

$$C_2=C_1+\left(\frac{1}{2}k_1+\frac{1}{2}k_2\right)h$$
$$=8.1205\times10^6+\left(\frac{1}{2}(-487230)+\frac{1}{2}(-384910)\right)3.5$$
$$=8.1205\times10^6+(-436070)3.5$$
$$=6.5943\times10^6\,\text{parts/m}^3$$

C_2 is the approximate concentration of bacteria at

$$t=t_2=t_1+h=3.5+3.5=7\,\text{weeks}$$

$$C(7)\approx C_2=6.5943\times10^6\ \text{parts/m}^3$$

Solution Cont

The exact solution of the ordinary differential equation is given by the solution of a non-linear equation as

$$C(t) = 1 \times 10^7 e^{\left(\frac{-3t}{50}\right)}$$

The solution to this nonlinear equation at t=7 weeks is

$$C(7) = 6.5705 \times 10^6 \text{ parts/m}^3$$

Runge-Kutta 4th Order Method

For $\qquad \dfrac{dy}{dx} = f(x,y), y(0) = y_0$

Runge Kutta 4th order method is given by

$$y_{i+1} = y_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h$$

where

$$k_1 = f\left(x_i, y_i\right)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right)$$

$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right)$$

$$k_4 = f\left(x_i + h, y_i + k_3 h\right)$$

Example

A ball at 1200K is allowed to cool down in air at an ambient temperature of 300K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067\times 10^{-12}\left(\theta^4 - 81\times 10^8\right), \theta(0) = 1200K$$

Find the temperature at $t = 480$ seconds using Runge-Kutta 4th order method.

Assume a step size of $h = 240$ seconds.

$$\frac{d\theta}{dt} = -2.2067\times 10^{-12}\left(\theta^4 - 81\times 10^8\right)$$

$$f(t,\theta) = -2.2067\times 10^{-12}\left(\theta^4 - 81\times 10^8\right)$$

$$\theta_{i+1} = \theta_i + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h$$

Solution

Step 1: $i = 0, t_0 = 0, \theta_0 = \theta(0) = 1200$

$$k_1 = f(t_0, \theta_o) = f(0,1200) = -2.2067\times10^{-12}\left(1200^4 - 81\times10^8\right) = -4.5579$$

$$k_2 = f\left(t_0 + \frac{1}{2}h, \theta_0 + \frac{1}{2}k_1 h\right) = f\left(0 + \frac{1}{2}(240), 1200 + \frac{1}{2}(-4.5579)240\right)$$
$$= f(120,653.05) = -2.2067\times10^{-12}\left(653.05^4 - 81\times10^8\right) = -0.38347$$

$$k_3 = f\left(t_0 + \frac{1}{2}h, \theta_0 + \frac{1}{2}k_2 h\right) = f\left(0 + \frac{1}{2}(240), 1200 + \frac{1}{2}(-0.38347)240\right)$$
$$= f(120,1154.0) = 2.2067\times10^{-12}\left(1154.0^4 - 81\times10^8\right) = -3.8954$$

$$k_4 = f(t_0 + h, \theta_0 + k_3 h) = f(0 + (240), 1200 + (-3.984)240)$$
$$= f(240,265.10) = 2.2067\times10^{-12}\left(265.10^4 - 81\times10^8\right) = 0.0069750$$

Solution Cont

$$\theta_1 = \theta_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$$= 1200 + \frac{1}{6}(-4.5579 + 2(-0.38347) + 2(-3.8954) + (0.069750))240$$

$$= 1200 + \frac{1}{6}(-2.1848)240$$

$$= 675.65K$$

θ_1 is the approximate temperature at

$$t = t_1 = t_0 + h = 0 + 240 = 240$$

$$\theta(240) \approx \theta_1 = 675.65K$$

Solution Cont

Step 2: $i = 1, t_1 = 240, \theta_1 = 675.65K$

$$k_1 = f(t_1, \theta_1) = f(240,675.65) = -2.2067\times10^{-12}\left(675.65^4 - 81\times10^8\right) = -0.44199$$

$$k_2 = f\left(t_1 + \frac{1}{2}h, \theta_1 + \frac{1}{2}k_1 h\right) = f\left(240 + \frac{1}{2}(240), 675.65 + \frac{1}{2}(-0.44199)240\right)$$
$$= f(360,622.61) = -2.2067\times10^{-12}\left(622.61^4 - 81\times10^8\right) = -0.31372$$

$$k_3 = f\left(t_1 + \frac{1}{2}h, \theta_1 + \frac{1}{2}k_2 h\right) = f\left(240 + \frac{1}{2}(240), 675.65 + \frac{1}{2}(-0.31372)240\right)$$
$$= f(360, 638.00) = 2.2067\times10^{-12}\left(638.00^4 - 81\times10^8\right) = -0.34775$$

$$k_4 = f(t_1 + h, \theta_1 + k_3 h) = f(240 + (240), 675.65 + (-0.34775)240)$$
$$= f(480,592.19) = 2.2067\times10^{-12}\left(592.19^4 - 81\times10^8\right) = -0.25351$$

Solution Cont

$$\theta_2 = \theta_1 + \frac{1}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)h$$

$$= 675.65 + \frac{1}{6}\left(-0.44199 + 2\left(-0.31372\right) + 2\left(-0.34775\right) + \left(-0.25351\right)\right)240$$

$$= 675.65 + \frac{1}{6}\left(-2.0184\right)240$$

$$= 594.91K$$

θ_2 is the approximate temperature at

$$t_2 = t_1 + h = 240 + 240 = 480$$

$$\theta(480) \approx \theta_2 = 594.91K$$

Solution Cont

The exact solution of the ordinary differential equation is given by the solution of a non-linear equation as

$$0.92593\ln\frac{\theta-300}{\theta+300}-1.8519\tan^{-1}\left(0.00333\theta\right)=-0.22067\times10^{-3}t-2.9282$$

The solution to this nonlinear equation at t=480 seconds is

$$\theta(480)=647.57K$$

Linear Solver

LU DECOMPOSITION

Overview

$$\begin{bmatrix} \alpha_{11} & 0 & 0 & 0 \\ \alpha_{21} & \alpha_{22} & 0 & 0 \\ \alpha_{31} & \alpha_{32} & \alpha_{33} & 0 \\ \alpha_{41} & \alpha_{42} & \alpha_{43} & \alpha_{44} \end{bmatrix} \cdot \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} & \beta_{14} \\ 0 & \beta_{22} & \beta_{23} & \beta_{24} \\ 0 & 0 & \beta_{33} & \beta_{34} \\ 0 & 0 & 0 & \beta_{44} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

$$i < j: \qquad \alpha_{i1}\beta_{1j} + \alpha_{i2}\beta_{2j} + \cdots + \alpha_{ii}\beta_{ij} = a_{ij} \tag{2.3.8}$$

$$i = j: \qquad \alpha_{i1}\beta_{1j} + \alpha_{i2}\beta_{2j} + \cdots + \alpha_{ii}\beta_{jj} = a_{ij} \tag{2.3.9}$$

$$i > j: \qquad \alpha_{i1}\beta_{1j} + \alpha_{i2}\beta_{2j} + \cdots + \alpha_{ij}\beta_{jj} = a_{ij} \tag{2.3.10}$$

$$\alpha_{ii} \equiv 1 \qquad i = 1, \ldots, N \tag{2.3.11}$$

Step 1

- Set $\alpha_{ii} = 1$, $i = 1, \ldots, N$ (equation 2.3.11).

This is handled implicitly in the code by only calculating the diagonal for β

Step 2

- For each $j = 1, 2, 3, \ldots, N$ do these two procedures: First, for $i = 1, 2, \ldots, j$, use (2.3.8), (2.3.9), and (2.3.11) to solve for β_{ij}, namely

$$\beta_{ij} = a_{ij} - \sum_{k=1}^{i-1} \alpha_{ik}\beta_{kj}. \tag{2.3.12}$$

(When $i = 1$ in 2.3.12 the summation term is taken to mean zero.) Second, for $i = j+1, j+2, \ldots, N$ use (2.3.10) to solve for α_{ij}, namely

$$\alpha_{ij} = \frac{1}{\beta_{jj}} \left(a_{ij} - \sum_{k=1}^{j-1} \alpha_{ik}\beta_{kj} \right). \tag{2.3.13}$$

Be sure to do both procedures before going on to the next j.

GAUSS ELIMINATION

Naïve Gaussian Elimination

A method to solve simultaneous linear equations of the form [A][X]=[C]

Two steps

1. Forward Elimination
2. Back Substitution

Forward Elimination

The goal of forward elimination is to transform the coefficient matrix into an upper triangular matrix

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Forward Elimination

A set of *n* equations and *n* unknowns

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = b_2$$

$$\begin{array}{cc} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{array}$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots + a_{nn}x_n = b_n$$

(n-1) steps of forward elimination

Forward Elimination

Step 1

For Equation 2, divide Equation 1 by a_{11} and multiply by a_{21}.

$$\left[\frac{a_{21}}{a_{11}}\right](a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1)$$

$$a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \ldots + \frac{a_{21}}{a_{11}}a_{1n}x_n = \frac{a_{21}}{a_{11}}b_1$$

Forward Elimination

Subtract the result from Equation 2.

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = b_2$$

$$- \quad a_{21}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \ldots + \frac{a_{21}}{a_{11}}a_{1n}x_n = \frac{a_{21}}{a_{11}}b_1$$

$$\left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \ldots + \left(a_{2n} - \frac{a_{21}}{a_{11}}a_{1n}\right)x_n = b_2 - \frac{a_{21}}{a_{11}}b_1$$

or $$a_{22}'x_2 + \ldots + a_{2n}'x_n = b_2'$$

Forward Elimination

Repeat this procedure for the remaining equations to reduce the set of equations as

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n = b'_2$$

$$a'_{32}x_2 + a'_{33}x_3 + \ldots + a'_{3n}x_n = b'_3$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$a'_{n2}x_2 + a'_{n3}x_3 + \ldots + a'_{nn}x_n = b'_n$$

End of Step 1

Forward Elimination

Step 2

Repeat the same procedure for the 3[rd] term of Equation 3.

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + \ldots + a''_{3n}x_n &= b''_3 \\
&\vdots \\
a''_{n3}x_3 + \ldots + a''_{nn}x_n &= b''_n
\end{aligned}
$$

End of Step 2

Forward Elimination

At the end of (n-1) Forward Elimination steps, the system of equations will look like

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + \ldots + a''_{3n}x_n &= b''_3 \\
\vdots \qquad & \quad \vdots \\
a_{nn}^{(n-1)}x_n &= b_n^{(n-1)}
\end{aligned}
$$

End of Step (n-1)

Matrix Form at End of Forward Elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ 0 & 0 & a''_{33} & \cdots & a''_{3n} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & a_{nn}^{(n-1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \\ \vdots \\ b_n^{(n-1)} \end{bmatrix}$$

Back Substitution

Solve each equation starting from the last equation

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.21 \\ 0.735 \end{bmatrix}$$

Example of a system of 3 equations

Back Substitution Starting Eqns

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n = b'_2$$

$$a''_{33}x_3 + \ldots + a''_{n}x_n = b''_3$$

$$\vdots \qquad \vdots$$

$$a_{nn}^{(n-1)}x_n = b_n^{(n-1)}$$

Back Substitution

Start with the last equation because it has only one unknown

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

Back Substitution

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

$$x_i = \frac{b_i^{(i-1)} - a_{i,i+1}^{(i-1)} x_{i+1} - a_{i,i+2}^{(i-1)} x_{i+2} - \ldots - a_{i,n}^{(i-1)} x_n}{a_{ii}^{(i-1)}} \text{ for } i = n-1,\ldots,1$$

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^{n} a_{ij}^{(i-1)} x_j}{a_{ii}^{(i-1)}} \text{ for } i = n-1,\ldots,1$$

Example 1

The upward velocity of a rocket is given at three different times

Table 1 Velocity vs. time data.

Time, $t\,(\mathrm{s})$	**Velocity,** $v\,(\mathrm{m/s})$
5	106.8
8	177.2
12	279.2

The velocity data is approximated by a polynomial as:

$$v(t) = a_1 t^2 + a_2 t + a_3 \;, \qquad 5 \le \mathrm{t} \le 12.$$

Find the velocity at t=6 seconds .

Example 1 Cont.

Assume

$$v(t) = a_1 t^2 + a_2 t + a_3 \ , \quad 5 \le t \le 12.$$

Results in a matrix template of the form:

$$\begin{bmatrix} t_1^2 & t_1 & 1 \\ t_2^2 & t_2 & 1 \\ t_3^2 & t_3 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

Using data from Table 1, the matrix becomes:

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Example 1 Cont.

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix} \Rightarrow \left[\begin{array}{ccccc} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{array}\right]$$

1. Forward Elimination
2. Back Substitution

Forward Elimination

Number of Steps of Forward Elimination

Number of steps of forward elimination is

$(n-1)=(3-1)=2$

Forward Elimination: Step 1

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 64 & 8 & 1 & \vdots & 177.2 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

Divide Equation 1 by 25 and

multiply it by 64, $\frac{.64}{25} = 2.56$

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \end{bmatrix} \times 2.56 = \begin{bmatrix} 64 & 12.8 & 2.56 & \vdots & 273.408 \end{bmatrix}$$

Subtract the result from Equation 2

$$\begin{array}{r} \begin{bmatrix} 64 & 8 & 1 & \vdots & 177.2 \end{bmatrix} \\ -\begin{bmatrix} 64 & 12.8 & 2.56 & \vdots & 273.408 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & -4.8 & -1.56 & \vdots & -96.208 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 2

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

Forward Elimination: Step 1 (cont.)

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 144 & 12 & 1 & \vdots & 279.2 \end{bmatrix}$$

Divide Equation 1 by 25 and

multiply it by 144, $\frac{144}{25} = 5.76$

$$[25 \quad 5 \quad 1 \quad \vdots \quad 106.8] \times 5.76 = [144 \quad 28.8 \quad 5.76 \quad \vdots \quad 615.168]$$

Subtract the result from Equation 3

$$\begin{array}{r} [144 \quad 12 \quad 1 \quad \vdots \quad 279.2] \\ -[144 \quad 28.8 \quad 5.76 \quad \vdots \quad 615.168] \\ \hline [0 \quad -16.8 \quad -4.76 \quad \vdots \quad -335.968] \end{array}$$

Substitute new equation for Equation 3

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & -16.8 & -4.76 & \vdots & -335.968 \end{bmatrix}$$

Forward Elimination: Step 2

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & -16.8 & -4.76 & \vdots & -335.968 \end{bmatrix}$$

Divide Equation 2 by −4.8

and multiply it by −16.8,

$$\frac{-16.8}{-4.8} = 3.5$$

$$\begin{bmatrix} 0 & -4.8 & -1.56 & \vdots & -96.208 \end{bmatrix} \times 3.5 = \begin{bmatrix} 0 & -16.8 & -5.46 & \vdots & -336.728 \end{bmatrix}$$

Subtract the result from Equation 3

$$\begin{array}{r} \begin{bmatrix} 0 & -16.8 & -4.76 & \vdots & 335.968 \end{bmatrix} \\ -\begin{bmatrix} 0 & -16.8 & -5.46 & \vdots & -336.728 \end{bmatrix} \\ \hline \begin{bmatrix} 0 & 0 & 0.7 & \vdots & 0.76 \end{bmatrix} \end{array}$$

Substitute new equation for Equation 3

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.208 \\ 0 & 0 & 0.7 & \vdots & 0.76 \end{bmatrix}$$

Back Substitution

Back Substitution

$$\begin{bmatrix} 25 & 5 & 1 & \vdots & 106.8 \\ 0 & -4.8 & -1.56 & \vdots & -96.2 \\ 0 & 0 & 0.7 & \vdots & 0.7 \end{bmatrix} \Rightarrow \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.208 \\ 0.76 \end{bmatrix}$$

Solving for a_3

$$0.7a_3 = 0.76$$

$$a_3 = \frac{0.76}{0.7}$$

$$a_3 = 1.08571$$

Back Substitution (cont.)

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.208 \\ 0.76 \end{bmatrix}$$

Solving for a_2

$$-4.8a_2 - 1.56a_3 = -96.208$$

$$a_2 = \frac{-96.208 + 1.56a_3}{-4.8}$$

$$a_2 = \frac{-96.208 + 1.56 \times 1.08571}{-4.8}$$

$$a_2 = 19.6905$$

Back Substitution (cont.)

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ -96.2 \\ 0.76 \end{bmatrix}$$

Solving for a_1

$$25a_1 + 5a_2 + a_3 = 106.8$$

$$\begin{aligned} a_1 &= \frac{106.8 - 5a_2 - a_3}{25} \\ &= \frac{106.8 - 5 \times 19.6905 - 1.08571}{25} \\ &= 0.290472 \end{aligned}$$

Naïve Gaussian Elimination Solution

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.290472 \\ 19.6905 \\ 1.08571 \end{bmatrix}$$

Example 1 Cont.

Solution

The solution vector is

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.290472 \\ 19.6905 \\ 1.08571 \end{bmatrix}$$

The polynomial that passes through the three data points is then:

$$\begin{aligned} v(t) &= a_1 t^2 + a_2 t + a_3 \\ &= 0.290472t^2 + 19.6905t + 1.08571, \quad 5 \le t \le 12 \end{aligned}$$

$$\begin{aligned} v(6) &= 0.290472(6)^2 + 19.6905(6) + 1.08571 \\ &= 129.686 \text{ m/s.} \end{aligned}$$